Computational Screening of Light-absorbing Materials for Photoelectrochemical Water Splitting
Efficient conversion of solar energy into electricity or fuels requires the identification of new semiconductors with optimal optical and electronic properties. We discuss the current and future role that computational screening is expected to play in this challenge. We discuss the identification of new computable descriptors characterising optimal materials performance, and we outline different search strategies in the materials screening. Finally, we describe some of the screening results obtained for perovskites, 2D materials, and for materials extracted from crystallographic databases.

Exploration versus Exploitation in Global Atomistic Structure Optimization
The ability to navigate vast energy landscapes of molecules, clusters, and solids is a necessity for discovering novel compounds in computational chemistry and materials science. For high-dimensional systems, it is only computationally feasible to search a small portion of the landscape, and hence, the search strategy is of critical importance. Introducing Bayesian optimization concepts in an evolutionary algorithm framework, we quantify the concepts of exploration and exploitation in global minimum searches. The method allows us to control the balance between probing unknown regions of the landscape (exploration) and investigating further regions of the landscape known to have low-energy structures (exploitation). The search for global minima structures proves significantly faster with the optimal balance for three test systems (molecular compounds) and to a lesser extent also for a crystalline surface reconstruction. In addition, global search behaviors are analyzed to provide reasonable grounds for an optimal balance for different problems.
High-Throughput Computational Assessment of Previously Synthesized Semiconductors for Photovoltaic and Photoelectrochemical Devices

Using computational screening we identify materials with potential use as light absorbers in photovoltaic or photoelectrochemical devices. The screening focuses on compounds of up to three different chemical elements which are abundant and nontoxic. A prescreening is carried out based on information from the Inorganic Crystal Structure Database and Open Quantum Materials Database. The light absorption, carrier mobility, defect tolerance, and stability of the materials are assessed by a set of simple computational descriptors. The identified 74 materials include a variety of pnictogenides, chalcogenides, and halides. Several recently investigated light absorbers, such as CsSnI₃, CsSnBr₃, and BaZrS₃, appear on the list.

General information
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Organisations: Department of Physics, Theoretical Atomic-scale Physics
Contributors: Kuhar, K., Pandey, M., Thygesen, K. S., Jacobsen, K. W.
Pages: 436-446
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ISSN (Print): 2380-8195
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Web of Science (2018): Indexed yes
Scopus rating (2017): CiteScore 10.24 SJR 5.991 SNIP 1.264
Web of Science (2017): Impact factor 12.277
Web of Science (2016): Impact factor
Web of Science (2015): Indexed yes
Original language: English
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Source: FindIt
Source-ID: 239556412
Research output: Research - peer-review » Journal article – Annual report year: 2018

Machine learning-based screening of complex molecules for polymer solar cells
Polymer solar cells admit numerous potential advantages including low energy payback time and scalable high-speed manufacturing, but the power conversion efficiency is currently lower than for their inorganic counterparts. In a Phenyl-C₆₁-Butyric-Acid-Methyl-Ester (PCBM)-based blended polymer solar cell, the optical gap of the polymer and the energetic alignment of the lowest unoccupied molecular orbital (LUMO) of the polymer and the PCBM are crucial for the device efficiency. Searching for new and better materials for polymer solar cells is a computationally costly affair using
density functional theory (DFT) calculations. In this work, we propose a screening procedure using a simple string representation for a promising class of donor-acceptor polymers in conjunction with a grammar variational autoencoder. The model is trained on a dataset of 3989 monomers obtained from DFT calculations and is able to predict LUMO and the lowest optical transition energy for unseen molecules with mean absolute errors of 43 and 74 meV, respectively, without knowledge of the atomic positions. We demonstrate the merit of the model for generating new molecules with the desired LUMO and optical gap energies which increases the chance of finding suitable polymers by more than a factor of five in comparison to the randomised search used in gathering the training set.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Cognitive Systems, Department of Energy Conversion and Storage, Atomic scale modelling and materials, Department of Physics, Theoretical Atomic-scale Physics
Contributors: Jørgensen, P. B., Mesta, M., Shil, S., García Lastra, J. M., Jacobsen, K. W., Thygesen, K. S., Schmidt, M. N.
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 2.5 SJR 1.252 SNIP 0.926
Web of Science (2017): Impact factor 2.843
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.13 SJR 1.486 SNIP 0.964
Web of Science (2016): Impact factor 2.965
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 1.98 SJR 1.255 SNIP 0.964
Web of Science (2015): Impact factor 2.894
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.54 SJR 1.446 SNIP 1.02
Web of Science (2014): Impact factor 2.952
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.95 SJR 1.559 SNIP 1.174
Web of Science (2013): Impact factor 3.122
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.86 SJR 1.832 SNIP 1.137
Web of Science (2012): Impact factor 3.164
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.07 SJR 1.845 SNIP 1.215
Web of Science (2011): Impact factor 3.333
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.777 SNIP 1.064
Promising quaternary chalcogenides as high-band-gap semiconductors for tandem photoelectrochemical water splitting devices: A computational screening approach

Significantly high efficiency of the photoelectrochemical (PEC) water splitting process can be achieved by using two semiconductors in a tandem device. The smaller band gap (SBG) material in the device has a band gap of similar to 1 eV, whereas the larger band gap (LBG) material has a band gap of similar to 2 eV. However, a very limited number of LBG semiconductors have been explored and here we investigate systematically the quaternary chalcogenides of A(2)BCX(4) type. We calculate the properties of the materials in six different crystal structures. Based on the criteria of thermodynamic stability, band gap, and good charge transport properties, we find a handful of potential LBG candidates from a pool of 1368 materials. Additionally, by extrapolating our analyses we also find a few SBG semiconductors, some of which are already known, e.g., CZTS/AgZTSe. This consolidates our approach for the LBG semiconductors and therefore invites experimental investigation of the candidates identified as efficient LBG semiconductors for the tandem devices.

General information
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Organisations: Department of Physics, Theoretical Atomic-scale Physics
Contributors: Pandey, M., Jacobsen, K. W.
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Publication information
Journal: Physical Review Materials
Volume: 2
Issue number: 10
Article number: 105402
Rich Ground State Chemical Ordering in Nanoparticles: Exact Solution of a Model for Ag-Au Clusters

We show that nanoparticles can have very rich ground state chemical order. This is illustrated by determining the chemical ordering of Ag-Au 309-atom Mackay icosahedral nanoparticles. The energy of the nanoparticles is described using a cluster expansion model, and a Mixed Integer Programming (MIP) approach is used to find the exact ground state configurations for all stoichiometries. The chemical ordering varies widely between the different stoichiometries, and display a rich zoo of structures with non-trivial ordering.

General information
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Organisations: Department of Physics, Theoretical Atomic-scale Physics
Contributors: Larsen, P. M., Jacobsen, K. W., Schiøtz, J.
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BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 7.58 SJR 3.622 SNIP 2.464
Web of Science (2017): Impact factor 8.839
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.33 SJR 4.196 SNIP 2.61
Web of Science (2016): Impact factor 8.462
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.76 SJR 4.656 SNIP 2.538
Web of Science (2015): Impact factor 7.645
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.62 SJR 5.232 SNIP 2.71
Web of Science (2014): Impact factor 7.512
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 7.46 SJR 5.675 SNIP 2.781
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 7.19 SJR 6.292 SNIP 2.867
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
The Computational 2D Materials Database: high-throughput modeling and discovery of atomically thin crystals

We introduce the Computational 2D Materials Database (C2DB), which organises a variety of structural, thermodynamic, elastic, electronic, magnetic, and optical properties of around 1500 two-dimensional materials distributed over more than 30 different crystal structures. Material properties are systematically calculated by state-of-the-art density functional theory and many-body perturbation theory (and the Bethe–Salpeter equation for ~250 materials) following a semi-automated workflow for maximal consistency and transparency. The C2DB is fully open and can be browsed online (http://c2db.fysik.dtu.dk) or downloaded in its entirety. In this paper, we describe the workflow behind the database, present an overview of the properties and materials currently available, and explore trends and correlations in the data. Moreover, we identify a large number of new potentially synthesizable 2D materials with interesting properties targeting applications within spintronics, (opto-)electronics, and plasmonics. The C2DB offers a comprehensive and easily accessible overview of the rapidly expanding family of 2D materials and forms an ideal platform for computational modeling and design of new 2D materials and van der Waals heterostructures.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Center for Nanostructured Graphene, Neutrons and X-rays for Materials Physics, Plasma Physics and Fusion Energy
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Publication date: 2018
Computational High-throughput Screening for Solar Energy Materials

State: Published
Organisations: Department of Energy Conversion and Storage, Department of Physics, Atomic scale modelling and materials, Theoretical Atomic-scale Physics
Contributors: Castelli, I. E., Thygesen, K. S., Jacobsen, K. W.
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Research output: Research - peer-review › Book chapter – Annual report year: 2017

Defect Chemistry and Electrical Conductivity of Sm-Doped La$_{1-x}$Sr$_x$CoO$_{3-\delta}$ for Solid Oxide Fuel Cells
We have calculated the electrical conductivity of the solid oxide fuel cell (SOFC) cathode contact material La$_{1-x}$Sr$_x$CoO$_{3-\delta}$ at 900 K. Experimental trends in conductivity against $x$, and against $\delta$ for fixed $x$, are correctly reproduced for $x \leq 0.8$. 

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Furthermore, we have studied the chemistry of neutral and charged intrinsic and extrinsic defects (dopants) in La$_{0.5}$Sr$_{0.5}$CoO$_3$ and have calculated the conductivity of the doped systems. In particular, we find that doping with Sm on the La site should enhance the conductivity, a prediction that is subsequently confirmed by electrical conductivity measurements.
Determination of low-strain interfaces via geometric matching

We present a general method for combining two crystals into an interface. The method finds all possible interfaces between the crystals with small coincidence cells and identifies the strain and area of the corresponding two-dimensional cells of the two crystal surfaces. We apply the method to the two semiconductor alloys InAs$_{1-x}$Sbx and Ga$_x$In$_{1-x}$As combined with a selection of pure metals or with NbTiN to create semiconductor/superconductor interfaces. The lattice constant of the alloy can be tuned by composition and we can extract the alloy lattice parameters corresponding to zero strain in both the metal and the alloy. The results can be used to suggest new epitaxially matched interfaces between two materials.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Neutrons and X-rays for Materials Physics, QuantumWise A/S
Contributors: Jelver, L., Larsen, P. M., Stradi, D., Stokbro, K., Jacobsen, K. W.
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Impact factor 3.813
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Impact factor 3.836
Web of Science (2016): Indexed yes
Scopus rating (2015): CiteScore 2.8 SJR 2.377 SNIP 1.13
Web of Science (2015): Impact factor 3.718
Web of Science (2015): Indexed yes
Scopus rating (2014): CiteScore 3.3 SJR 2.762 SNIP 1.316
Dynamic breaking of a single gold bond

While one might assume that the force to break a chemical bond gives a measure of the bond strength, this intuition is
misleading. If the force is loaded slowly, thermal fluctuations may break the bond before it is maximally stretched, and the
breaking force will be less than the bond can sustain. Conversely, if the force is loaded rapidly it is more likely that the
maximum breaking force is measured. Paradoxically, no clear differences in breaking force were observed in experiments
on gold nanowires, despite being conducted under very different conditions. Here we explore the breaking behaviour of a
single Au-Au bond and show that the breaking force is dependent on the loading rate. We probe the temperature and
structural dependencies of breaking and suggest that the paradox can be explained by fast breaking of atomic wires and slow breaking of point contacts giving very similar breaking forces.

**General information**

State: Published

Organisations: Department of Physics, Theoretical Atomic-scale Physics, University of Bern, University of Copenhagen


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Peer-reviewed: Yes

**Publication information**

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BFI (2018): BFI-level 2

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BFI (2017): BFI-level 2

Scopus rating (2017): CiteScore 12.41 SJR 6.582 SNIP 2.912

Web of Science (2017): Impact factor 12.353

Web of Science (2017): Indexed yes

BFI (2016): BFI-level 2

Scopus rating (2016): CiteScore 11.8 SJR 6.414 SNIP 2.855

Web of Science (2016): Impact factor 12.124

Web of Science (2016): Indexed yes

BFI (2015): BFI-level 1

Scopus rating (2015): CiteScore 11.23 SJR 6.287 SNIP 2.86


Web of Science (2015): Indexed yes

BFI (2014): BFI-level 1

Scopus rating (2014): CiteScore 10.77 SJR 6.41 SNIP 3.034

Web of Science (2014): Impact factor 11.47

Web of Science (2014): Indexed yes

BFI (2013): BFI-level 1

Scopus rating (2013): CiteScore 9.85 SJR 6.206 SNIP 2.797

Web of Science (2013): Impact factor 10.742

ISI indexed (2013): ISI indexed yes

Web of Science (2013): Indexed yes

Scopus rating (2012): CiteScore 8.32 SJR 5.866 SNIP 2.829

Web of Science (2012): Impact factor 10.015

ISI indexed (2012): ISI indexed yes

Web of Science (2012): Indexed yes

Scopus rating (2011): CiteScore 4.44 SJR 3.137 SNIP 1.825

Web of Science (2011): Impact factor 7.396

ISI indexed (2011): ISI indexed no

Web of Science (2010): Impact factor

Web of Science (2010): Indexed yes

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Source: FindIt

Source-ID: 2372367346

Research output: Research - peer-review ; Journal article – Annual report year: 2017
Effect of edge plasmons on the optical properties of MoS$_2$ monolayer flakes

Finite MoS$_2$ nanoparticles are known to support metallic edge states that are responsible for their catalytic activity. In this work we employ time-dependent density-functional theory (TDDFT) to study the influence of such edge states on the optical properties of triangular MoS$_2$ monolayer flakes. We find that the edge states support collective plasmon-like excitations that couple strongly to the optical field leading to pronounced absorption peaks below the onset of interband transitions on the basal plane. Additionally, structural relaxation of the flakes can significantly distort the edge states. Thus, we observe that while an evenly-spaced edge configuration supports one-dimensional (1D) plasmon modes similar to those of an ideal 1D electron gas, the relaxed structures show mixed plasmon and single-electron excitations in the low-energy response. Our findings illustrate the sensitivity of the optical response of MoS$_2$ nanostructures to the details of the edge configuration.

General information
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Article number: 155407
ISSN (Print): 2469-9950
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Impact factor 3.813
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Impact factor 3.836
Web of Science (2016): Indexed yes
Scopus rating (2015): CiteScore 2.8 SJR 2.377 SNIP 1.13
Web of Science (2015): Impact factor 3.718
Web of Science (2015): Indexed yes
Scopus rating (2014): CiteScore 3.3 SJR 2.762 SNIP 1.316
Web of Science (2014): Impact factor 3.736
Web of Science (2014): Indexed yes
Scopus rating (2013): CiteScore 3.55 SJR 2.813 SNIP 1.326
Web of Science (2013): Impact factor 3.664
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): CiteScore 3.57 SJR 3.173 SNIP 1.378
Web of Science (2012): Impact factor 3.767
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): CiteScore 3.61 SJR 3.326 SNIP 1.423
Web of Science (2011): Impact factor 3.691
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 3.318 SNIP 1.447
Web of Science (2010): Impact factor 3.774
Web of Science (2010): Indexed yes
Grid-Based Projector Augmented Wave (GPAW) Implementation of Quantum Mechanics/Molecular Mechanics (QM/MM) Electrostatic Embedding and Application to a Solvated Diplatinum Complex

A multiscale density functional theory-quantum mechanics/molecular mechanics (DFT-QM/MM) scheme is presented, based on an efficient electrostatic coupling between the electronic density obtained from a grid-based projector augmented wave (GPAW) implementation of density functional theory and a classical potential energy function. The scheme is implemented in a general fashion and can be used with various choices for the descriptions of the QM or MM regions. Tests on H2O clusters, ranging from dimer to decamer show that no systematic energy errors are introduced by the coupling that exceeds the differences in the QM and MM descriptions. Over 1 ns of liquid water, Born-Oppenheimer QM/MM molecular dynamics (MD) are sampled combining 10 parallel simulations, showing consistent liquid water structure over the QM/MM border. The method is applied in extensive parallel MD simulations of an aqueous solution of the diplatinum [Pt2(P2O5H2)4]- complex (PtPOP), spanning a total time period of roughly half a nanosecond. An average Pt-Pt distance deviating only 0.01 Å from experimental results, and a ground-state Pt-Pt oscillation frequency deviating by

General information
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Organisations: Department of Chemistry, Department of Physics, Theoretical Atomic-scale Physics, NanoChemistry, University of Iceland, Aalto University
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Publication date: 2017
Peer-reviewed: Yes

Publication information
Journal: Journal of Chemical Theory and Computation
Volume: 13
Issue number: 12

Recent experiments on II–IV–V₂ type nitrides and phosphides have shown that these materials are potential candidates as photovoltaic absorbers. The materials space for such light absorbers can be expanded by elemental substitution of the different species, and thanks to the small energy difference of the polymorphs, the space can be extended by tuning the atomic structure as well. Using electronic structure calculations, we explore chalcopyrite, kesterite, and wurtzite polymorphs of II–IV–V₂ and III–III–V₂ materials for light absorption especially in the visible range. Based on the thermodynamic stability, band gap, and charge carrier effective masses, we discuss the possibility for the materials containing nontoxic elements to act as PV absorbers. Additionally, the systematic mapping of the materials space provides trends in thermodynamic and electronic properties which can be exploited further to tune these properties via elemental substitution and/or alloying.

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Organisations: Department of Physics, Theoretical Atomic-scale Physics
Contributors: Pandey, M., Kuhar, K., Jacobsen, K. W.
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Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry C
Volume: 121
Issue number: 33
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
Web of Science (2017): Impact factor 4.484
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195
Web of Science (2016): Impact factor 4.536
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4.68 SJR 1.886 SNIP 1.26
Web of Science (2015): Impact factor 4.509
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 5.08 SJR 2.032 SNIP 1.447
Web of Science (2014): Impact factor 4.772
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 5.14 SJR 2.143 SNIP 1.445
Web of Science (2013): Impact factor 4.835
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 4.98 SJR 2.529 SNIP 1.461
Web of Science (2012): Impact factor 4.814
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 4.92 SJR 2.339 SNIP 1.465
Web of Science (2011): Impact factor 4.805
ISI indexed (2011): ISI indexed yes
Roughness in flatland

Energy-favoured grain rotation in nanocrystalline metals is shown to cause surface roughness at the atomic scale, providing fundamental insight for grain boundary engineering in materials design.
Sulfide perovskites for solar energy conversion applications: computational screening and synthesis of the selected compound LaYS\textsubscript{3}

One of the key challenges in photoelectrochemical water splitting is to identify efficient semiconductors with band gaps of the order of ∼2 eV to operate as the large-band-gap component in water splitting tandem devices. Here, we address this challenge by extensive computational screening of ternary sulfides followed by synthesis and confirmation of the properties of one of the most promising materials. The screening focuses on materials with ABS\textsubscript{3} composition taking both perovskite and non-perovskite structures into consideration, and the material selection is based on descriptors for thermodynamic stability, light absorption, charge mobility, and defect tolerance. One of the most promising candidates identified is LaYS\textsubscript{3}. This material was synthesized directly in thin-film form demonstrating its stability, crystal structure, light absorption, and strong photoluminescence. These data confirms its potential applicability in tandem photoelectrochemical devices for hydrogen production.
Sustainable solar fuels and electricity through discovery and prototyping of new materials

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Silicon Microtechnology, Theoretical Atomic-scale Physics, Department of Micro- and Nanotechnology
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Publisher: Technical University of Denmark (DTU)
Article number: M-1
Electronic versions: SustainAbstracts2017c.compressed_115.pdf

The Atomic Simulation Environment - A Python library for working with atoms
The Atomic Simulation Environment (ASE) is a software package written in the Python programming language with the aim of setting up, steering, and analyzing atomistic simulations. In ASE, tasks are fully scripted in Python. The powerful syntax of Python combined with the NumPy array library make it possible to perform very complex simulation tasks. For example, a sequence of calculations may be performed with the use of a simple "for-loop" construction. Calculations of energy, forces, stresses and other quantities are performed through interfaces to many external electronic structure codes or force fields using a uniform interface. On top of this calculator interface, ASE provides modules for performing many standard simulation tasks such as structure optimization, molecular dynamics, handling of constraints and performing nudged elastic band calculations.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Department of Energy Conversion and Storage, Atomic scale modelling and materials, Department of Micro- and Nanotechnology, Theoretical Nanotechnology, University of Barcelona, University of Copenhagen, Malmö University, SINTEF, Aarhus University, Brown University, University of Wisconsin-Madison, University of Warwick, Carnegie Mellon University, Purdue University, Siminn, Karlsruhe Institute of Technology, Swiss Federal Institute of Technology Zurich, University of Freiburg
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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.37 SJR 0.875 SNIP 0.921
Web of Science (2017): Impact factor 2.617
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.89 SJR 1.553 SNIP 0.91
Atomically Thin Ordered Alloys of Transition Metal Dichalcogenides: Stability and Band Structures

We explore the possibility of modulating the electronic band edges of the transition metal dichalcogenides (TMD) via alloying of different semiconductors within the same group (intra-group alloying). The stability of the ordered alloys is assessed from the calculated mixing enthalpy which is found to be close to zero for several alloys and below 20 meV/atom for all the alloys. We explore to what extent the electronic properties like the band gap and band edge positions of the alloy can be evaluated by taking the weighted average of the corresponding properties of the pristine systems. In general, this approach works well with the only exception being Cr containing compounds. Because the calculated properties of the alloys are very similar to the weighted averages, we expect that the trends observed for the ordered alloys will also hold for more realistic disordered alloys.
Band Gap Tuning and Defect Tolerance of Atomically Thin Two-Dimensional Organic-Inorganic Halide Perovskites

Organic–inorganic halide perovskites have proven highly successful for photovoltaics but suffer from low stability, which deteriorates their performance over time. Recent experiments have demonstrated that low dimensional phases of the hybrid perovskites may exhibit improved stability. Here we report first-principles calculations for isolated monolayers of the organometallic halide perovskites \((\text{C}_4\text{H}_9\text{NH}_3)_2\text{MX}_2\text{Y}_2\), where \(M = \text{Pb, Ge, Sn}\) and \(X, Y = \text{Cl, Br, I}\). The band gaps computed using the GLLB-SC functional are found to be in excellent agreement with experimental photoluminescence data for the already synthesized perovskites. Finally, we study the effect of different defects on the band structure. We find that the most common defects only introduce shallow or no states in the band gap, indicating that these atomically thin 2D perovskites are likely to be defect tolerant.

General information
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Organisations: Department of Physics, Theoretical Atomic-scale Physics, Center for Nanostructured Graphene
Contributors: Pandey, M., Jacobsen, K. W., Thygesen, K. S.
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Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
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Localized electronic states formed inside the band gap of a semiconductor due to crystal defects can be detrimental to the material's optoelectronic properties. Semiconductors with a lower tendency to form defect induced deep gap states are termed defect-tolerant. Here we provide a systematic first-principles investigation of defect tolerance in 29 monolayer transition metal dichalcogenides (TMDs) of interest for nanoscale optoelectronics. We find that the TMDs based on group
VI and X metals form deep gap states upon creation of a chalcogen (S, Se, Te) vacancy, while the TMDs based on group IV metals form only shallow defect levels and are thus predicted to be defect-tolerant. Interestingly, all the defect sensitive TMDs have valence and conduction bands with a very similar orbital composition. This indicates a bonding/antibonding nature of the gap, which in turn suggests that dangling bonds will fall inside the gap. These ideas are made quantitative by introducing a descriptor that measures the degree of similarity of the conduction and valence band manifolds. Finally, the study is generalized to nonpolar nanoribbons of the TMDs where we find that only the defect sensitive materials form edge states within the band gap.
Making the most of materials computations

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mBEEF-vdW: Robust fitting of error estimation density functionals

We propose a general-purpose semilocal/nonlocal exchange-correlation functional approximation, named mBEEF-vdW. The exchange is a meta generalized gradient approximation, and the correlation is a semilocal and nonlocal mixture, with the Rutgers-Chalmers approximation for van der Waals (vdW) forces. The functional is fitted within the Bayesian error estimation functional (BEEF) framework [J. Wellendorff et al., Phys. Rev. B 85, 235149 (2012); J. Wellendorff et al., J. Chem. Phys. 140, 144107 (2014)]. We improve the previously used fitting procedures by introducing a robust MM-estimator based loss function, reducing the sensitivity to outliers in the datasets. To more reliably determine the optimal model complexity, we furthermore introduce a generalization of the bootstrap 0.632 estimator with hierarchical bootstrap sampling and geometric mean estimator over the training datasets. Using this estimator, we show that the robust loss function leads to a 10% improvement in the estimated prediction error over the previously used least-squares loss function. The mBEEF-vdW functional is benchmarked against popular density functional approximations over a wide range of datasets relevant for heterogeneous catalysis, including datasets that were not used for its training. Overall, we find that mBEEF-vdW has a higher general accuracy than competing popular functionals, and it is one of the best performing functionals on chemisorption systems, surface energies, lattice constants, and dispersion. We also show the potential-energy curve of graphene on the nickel(111) surface, where mBEEF-vdW matches the experimental binding length. mBEEF-vdW is currently available in GPAW and other density functional theory codes through Libxc, version 3.0.0.
Anharmonic stabilization and band gap renormalization in the perovskite CsSnI$_3$

Amongst the X(Sn,Pb)Y$_3$ perovskites currently under scrutiny for their photovoltaic applications, the cubic B−α phase of CsSnI$_3$ is arguably the best characterized experimentally. Yet, according to the standard harmonic theory of phonons, this deceptively simple phase should not exist at all due to rotational instabilities of the SnI$_6$ octahedra. Here, employing self-consistent phonon theory, we show that these soft modes are stabilized at experimental conditions through anharmonic phonon-phonon interactions between the Cs ions and their iodine cages. We further calculate the renormalization of the electronic energies due to vibrations and find an unusual opening of the band gap, estimated as 0.24 and 0.11 eV at 500 and 300 K, which we attribute to the stretching of Sn-I bonds. Our work demonstrates the important role of temperature in accurately describing these materials.
Band-gap engineering of functional perovskites through quantum confinement and tunneling

An optimal band gap that allows for a high solar-to-fuel energy conversion efficiency is one of the key factors to achieve sustainability. We investigate computationally the band gaps and optical spectra of functional perovskites composed of layers of the two cubic perovskite semiconductors BaSnO3 and BaTaO2N. Starting from an indirect gap of around 3.3 eV for BaSnO3 and a direct gap of 1.8 eV for BaTaO2N, different layerings can be used to design a direct gap of the functional perovskite between 2.3 and 1.2 eV. The variations of the band gap can be understood in terms of quantum confinement and tunneling. We also calculate the light absorption of the different heterostructures and demonstrate a large sensitivity to the detailed layering.
We present calculations of the optical properties of a set of around 80 oxides, oxynitrides, and organometal halide cubic and layered perovskites (Ruddlesden-Popper and Dion-Jacobson phases) with a bandgap in the visible part of the solar spectrum. The calculations show that for different classes of perovskites the solar light absorption efficiency varies greatly depending not only on bandgap size and character (direct/indirect) but also on the dipole matrix elements. The oxides exhibit generally a fairly weak absorption efficiency due to indirect bandgaps while the most efficient absorbers are found in the classes of oxynitride and organometal halide perovskites with strong direct transitions.
Computational design of molecules for dye sensitized solar cells and nano electronics

The huge increase in computational power has enabled the use of high-throughput computational screening methods for many purposes. In combination with more detailed computational studies, this provides a powerful tool in the search for new materials and molecules useful for e.g. photovoltaics. This is illustrated in this thesis, where a high-throughput Density Functional Theory study of a total of 5145 porphyrin based dye molecules is presented. Initially, the structures of the dyes are optimized and the frontier energy orbital energies calculated. Following this, the dyes are scored for use in a dye sensitized solar cell (DSSC) in terms of a loss-less level alignment quality. This scoring only takes into account a simplified absorption spectrum of the dye in combination with the alignment between the molecular levels, the semi-conductor conduction band edge and the redox mediator. To improve on this, the effect of the free energy barrier associated with the dye regeneration reaction is included through extensive molecular dynamics simulations for a simple model dye, followed by an extrapolation of the result to the 5145 porphyrins. This model succeeds in rediscovering high efficiency dyes and suggests that the next generation of high efficiency porphyrin dyes may utilize a titanium metal center. Furthermore, the large internal reorganization energies calculated for the octahedral cobalt complexes, used as redox mediators, lead to the requirement of a large driving force for the regeneration reaction. Hence, using redox mediators with a lower internal reorganization energy would allow for a less constrained choice of dye, possibly boosting the efficiency.

The obtained data is furthermore used to search for suitable pairs of porphyrins for a novel type of DSSC schemes, using two dyes in a molecular two-photon tandem approach. Here, a high current is sacrificed for a larger voltage. As a smaller current is however often associated with a better fill-factor, the proposed scheme may lead to an increase in the efficiency. Specific candidates for the different schemes are identified and the resulting setups have theoretically obtainable open-circuit voltages exceeding 1.5 V.

Creating a metal-molecule-metal junction allows tuning the conductance through the junction by manipulating the molecular energy levels. In this thesis a computational approach to model the conductance as a function of the applied bias voltage, shifting the molecular levels, for a redox active molecule is presented and compared to experimental results. Here, it is shown that shifting the molecular energy levels in, out of resonance with the Fermi level of the electrodes, allows for a standard tuning of the conductance. In addition to this, reversibly changing the redox state, allows for switching quantum interference on and off, shifting the conductance by an order of magnitude. The simple computational model used is furthermore qualitatively found to be in very good agreement with experiments.

A different way of tuning the conductance through a molecular junction, is by controlling the junction geometry. This is achieved by designing a molecule with two sets of anchor groups, which bind to gold with significantly different strengths. Hence, it is proposed that the geometry can be controlled by chemical passivisation of one type of anchor group. Using a simple computational model, this experimental hypothesis is verified and the change in conductance upon changing junction geometry is reproduced.
Computational Screening of Energy Materials
The current energy consumption of the world's population relies heavily on fossil fuels. Unfortunately, the consumption of fossil fuels not only results in the emission of greenhouse gases which have deleterious effects on the environment but also the fossil fuel reserve is limited. Therefore, it is the need of the hour to search for environmentally benign renewable energy resources. The biggest source of the renewable energy is our sun and the immense energy it provides can be used to power the whole planet. However, an efficient way to harvest the solar energy to meet all the energy demand has not been realized yet.

A promising way to utilize the solar energy is the photon assisted water splitting. The process involves the absorption of sunlight with a semiconducting material (or a photoabsorber) and the generated electron-hole pair can be used to produce hydrogen by splitting the water. However, a single material cannot accomplish the whole process of the hydrogen evolution. In order to do so, a material should be able to absorb the sunlight and generate the electron-hole pairs and evolve hydrogen at the cathode and oxygen at anode using the generated electron and hole respectively.

This thesis using first-principle calculations explores materials for the light absorption with the bandgap, band edge positions and the stability in aqueous conditions as descriptors. This strategy results in a handful of materials which can act as good photoabsorbers for the water splitting reaction. Additionally, strategies to tune the bandgap for different applications is also explored. To carry out the cathode reaction, two-dimensional metal dichalcogenides and oxides are explored with a suggestion of few potential candidates for the hydrogen evolution reaction.

The thermodynamics of all the above process requires an accurate description of the energies with the first-principle calculations. Therefore, along this line the accuracy and predictability of the Meta-Generalized Gradient Approximation functional with Bayesian error estimation is also assessed.

Heats of formation of solids with error estimation: The mBEEF functional with and without fitted reference energies
The need for prediction of accurate electronic binding energies has led to the development of different schemes for combining density functional calculations, typically at the level of the generalized gradient approximation (GGA), with experimental information. We analyze one such scheme by Stevanovic et al. [Phys. Rev. B85, 115104 (2012);PRBMD098:012110.1103/PhysRevB.85:115104] for predictions of compound enthalpies of formation using fitted elemental-phase reference energies. We show that different versions of GGA with or without +U and a meta-GGA (TPSS) lead to comparable accuracy after fitting the reference energies. Our results also show that the recently developed mBEEF, a Bayesian error estimation functional, gives comparable accuracy with the other functionals even without the fitting. The mBEEF functional furthermore supplies an ensemble estimate of the prediction errors in reasonable agreement with the actual errors. We also show that using the fitting scheme on the mBEEF ensemble leads to improved accuracy including realistic error estimation.
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Importance of the Reorganization Energy Barrier in Computational Design of Porphyrin-Based Solar Cells with Cobalt-Based Redox Mediators

The shift from iodide-based redox mediators in dye-sensitized solar cells toward octahedral cobalt complexes has led to a significant increase in the efficiency. However, due to the nature of this type of complexes the driving force required for the regeneration of the dye is very high, and this limits the achievable efficiency. Here we show that the large driving force is a direct consequence of the large reorganization energy of the dye regeneration reaction. The reorganization energies for charge transfer between a simple zinc porphyrin dye and two popular cobalt-based redox mediators is calculated using ab initio molecular dynamics with explicit solvent. These results are then combined with a Marcus-based extrapolation scheme to obtain the reorganization energies of more than 5000 porphyrin-based dyes. We propose a scheme for scoring the performance of the porphyrin dyes, which is able to identify already known high-performance dyes in addition to a number of even better candidates. Our analysis shows that the large internal reorganization energy of the Co-based redox mediators is an obstacle for achieving higher efficiencies.

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Quantum theory of plasmons in nanostructures

In this thesis, *ab initio* quantum-mechanical calculations are used to study the properties of plasmons in nanostructures that involve atomic length-scales. The plasmon is an electronic excitation that corresponds to oscillations in the electron charge density in metals, often visualized as water ripples in a pond where the water represents a sea of free electrons. Plasmons on metal surfaces and in nanostructured materials, such as metal nanoparticles and atomically thin two-dimensional materials, have several technological applications due to their ability to confine light on nanoscale.

For a theoretical description of plasmon in such materials, where the electrons are heavily confined in one or more directions, a quantum mechanical description of the electrons in the material is necessary. In this thesis, the *ab initio* methods Density functional theory (DFT) and linear response time-dependent DFT are applied to calculate the properties of plasmons in nanostructures in different dimensions. In order to identify and visualize localized plasmon modes, a method for calculating plasmon eigenmodes within the *ab initio* framework has been developed. In the studied materials, quantum mechanical effects such as coupling to single-electronic transitions, electron spill-out from the surface, tunneling, and spatial non-locality, are shown to alter the plasmon excitations.

The studied systems include two-dimensional materials, such as thin metal films, monolayer transition metal dichalcogenides, and graphene. Here, also van der Waals heterostructures (vdWh), which are stacks of different twodimensional materials, are considered. A new multi-scale approach for calculating the dielectric-function of vdWh, which extends *ab initio* accuracy to the description of hundreds of atomic layers, is presented. Also, one-dimensional plasmons are studied in the case of atomically thin nanowires and edge-states of MoS$_2$. 
Strain sensitivity of band gaps of Sn-containing semiconductors

Tuning of band gaps of semiconductors is a way to optimize materials for applications within photovoltaics or as photocatalysts. One way to achieve this is through applying strain to the materials. We investigate the effect of strain on a range of Sn-containing semiconductors using density functional theory and many-body perturbation theory calculations. We find that the band gaps of bulk Sn oxides with SnO$_6$ octahedra are highly sensitive to volumetric strain. By applying a small isotropic strain of 2% (-2%), a decrease (increase) of band gaps as large as 0.8 to 1.0 eV are obtained. We attribute the ultrahigh strain sensitivity to the pure Sn s-state character of the conduction-band edges. Other Sn-containing compounds may show both increasing and decreasing gaps under tensile strain and we show that the behavior can be understood by analyzing the role of the Sn s states in both the valence and the conduction bands.
We explore the possibilities of hydrogen evolution by basal planes of 2D metal dichalcogenides and oxides in the 2H and 1T class of structures using the hydrogen binding energy as a computational activity descriptor. For some groups of systems like the Ti, Zr, and Hf dichalcogenides the hydrogen bonding to the 2H structure is stronger than that to the 1T structure, while for the Cr, Mo, and W dichalcogenides the behavior is opposite. This is rationalized by investigating shifts in the chalcogenide p levels comparing the two structures. We find that usually for a given material only at most one of the two phases will be active for the hydrogen evolution reaction; however, in most cases the two phases are very close in formation energy, opening up the possibility for stabilizing the active phase. The study points to many new possible 2D HER materials beyond the few that are already known.
Using Protection Layers for a 2-Photon Water Splitting Device

The 2-photon tandem device for photocatalytic water splitting has been theoretically shown to provide a higher efficiency than a single photon device (1). This increased efficiency can be achieved by having one material optimized to absorb high energy photons (large bandgap) and another material optimized to absorb low energy photons (small bandgap). To a large degree this approach has been hindered by corrosion issues. In this talk I will first discuss how our computational screening of 2,400 materials showed that very few materials can efficiently absorb light without corroding in water splitting conditions (2). I will follow this up by discussing how protection layers bypass the corrosion issue by creating a buffer layer (3). Finally I will show how we integrated a photocatalyst/protection layer/co-catalyst scheme to produce highly efficient H2 evolution photocathodes and O2 evolution photoanodes (3, 4). 1. A. B. Laursen, S. Kegnaes, S. Dahl and I. Chorkendorff, Energy & Environmental Science, 5 (2012). 2. B. Seger, I. E. Castelli, P. C. K. Vesborg, K. W. Jacobsen, O. Hansen and I. Chorkendorff, Energy & Environmental Science, 7, 2397 (2014). 3. B. Seger, T. Pedersen, A. B. Laursen, P. C. K. Vesborg, O. Hansen and I. Chorkendorff, Journal of the American Chemical Society, 135, 1057 (2013). 4. B. Mei, A. A. Permyakova, R. Frydendal, D. Bae, T. Pedersen, P. Malacrida, O. Hansen, I. E. L. Stephens, P. C. K. Vesborg, B. Seger and I. Chorkendorff, The Journal of Physical Chemistry Letters, 5, 3456 (2014). [Figure]
protection layer in conjunction with known H-2 evolution catalysts, protection is clearly feasible for a large bandgap photocathode. This suggests that there may be promising strategies for photocatalytic water splitting by using a large bandgap photocathode and a low bandgap photoanode with attached protection layers.
Assessing the reliability of calculated catalytic ammonia synthesis rates

We introduce a general method for estimating the uncertainty in calculated materials properties based on density functional theory calculations. We illustrate the approach for a calculation of the catalytic rate of ammonia synthesis over a range of transition-metal catalysts. The correlation between errors in density functional theory calculations is shown to play an important role in reducing the predicted error on calculated rates. Uncertainties depend strongly on reaction conditions and catalyst material, and the relative rates between different catalysts are considerably better described than the absolute rates. We introduce an approach for incorporating uncertainty when searching for improved catalysts by evaluating the probability that a given catalyst is better than a known standard.

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Bandgap calculations and trends of organometal halide perovskites

Energy production from the Sun requires a stable efficient light absorber. Promising candidates in this respect are organometal perovskites (ABX₃), which have been intensely investigated during the last years. Here, we have performed electronic structure calculations of 240 perovskites composed of Cs, CH₃NH₃, and HC(NH₂)₂ as A-cation, Sn and Pb as B-ion, and a combination of Cl, Br, and I as anions. The calculated gaps span over a region from 0.5 to 5.0 eV. In addition, the trends over bandgaps have been investigated: the bandgap increases with an increase of the electronegativities of the constituent species, while it reduces with an increase of the lattice constants of the system.
Calculated Pourbaix Diagrams of Cubic Perovskites for Water Splitting: Stability Against Corrosion

We use density functional theory calculations to investigate the stability of cubic perovskites for photo-electrochemical water splitting taking both materials in their bulk crystal structure and dissolved phases into account. The method is validated through a detailed comparison of the calculated and experimental Pourbaix diagrams for TiO2 and ZnO. For a class of 23 oxides, oxynitrides, and oxyfluorides, which were recently proposed as candidates for one-photon water splitting, our calculations predict most of the materials to be stable at potentials around the water red-ox level. The oxides become less stable at lower potentials, while the oxynitrides become unstable at higher potentials. We discuss the implications of these findings for the problem of photo-corrosion of water splitting electrodes.

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Designing rules and probabilistic weighting for fast materials discovery in the Perovskite structure.

High-throughput electronic-structure calculations are becoming increasingly popular in materials science and in the design of new compounds. Electronic-structure theory, for example, in the form of density-functional theory, can be used to calculate stabilities and electronic properties as bandgaps of new compounds. However, in practice, the methods are often limited to rather small atomic-scale systems or periodic crystals with only a limited number of atoms in the unit cell. It is therefore of interest to be able to derive generally useful information from simple systems to be applied in other, more complex, crystals. Here, we consider a large database of calculated stabilities and bandgaps of oxides and oxynitrides in the perovskite structure. We use the database as a testing ground for existing ideas about the behavior of these types of compounds and we derive some new simple chemical-based rules which combine structural information, like the ionic radii of the chemical elements, with electronic data, like the number of electrons and the valences of the pure elements. The rules extracted from the ABO$_3$ cubic perovskite are then tested using the ABO$_2$N and A$_2$BO$_4$ stoichiometry in the cubic and layered perovskite structure, respectively. These rules allow a saving in computer time of around 80%.

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Development and testing of new exchange correlation functionals
Catalysts are used in 90% of the world’s chemical processes to produce 60% of its chemical products, and they are thus very important to our modern society. We therefore seek to better understand current catalytic materials, so that we can find alternatives that will improve the energy efficiency, selectivity or similar of current chemical processes, or to make new technologies economical feasible. Kohn-Sham density functional theory (KS-DFT) has proven to be a powerful theory to find trends in current catalytic materials, which can empower a more informed search for better alternatives. KS-DFT relies on accurate and efficient approximations to the exchange correlation functional, yet these functional approximations have lacked a systematic way to estimate the underlying uncertainties. A Bayesian error estimation approach provides a mechanism for calculating approximative uncertainties, and so accurate, computationally feasible exchange-correlation approximations that incorporate it have been called for. This thesis presents significant steps forwards towards providing general applicable exchange-correlation functional approximations with Bayesian error estimation capabilities. A semi-empirical approach was used with a machine learning toolset to improve accuracy and transferability of the functional approximations. The toolset includes Tikhonov regularization of smoothness in a transformed model space, for ensuring sensible model solutions; an explicit model compromise with a geometric mean loss function, for ensuring generally applicable models; a robust MM-estimator loss function, for ensuring resistance to outliers in data; and a hierarchical bootstrap resampling estimating prediction error validation method, for selecting the model complexity that provide best transferability outside the training data. Three new semi-empirical functional approximations have been made: BEEF-vdW, mBEEF, and mBEEFvdW. It is shown that these functionals are able balance the accuracy of predicting energetics of covalent and non-covalent chemistry better than any comparative functional that we have tested, and they could therefore become the functional approximations of choice for understanding chemical processes at the solid-gas and solid-liquid interfaces.

General information
State: Published
Organisations: Department of Physics
Contributors: Lundgård, K. T., Jacobsen, K. W., Thygesen, K. S., Bligaard, T.
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Direct Dynamics Studies of a Binuclear Metal Complex in Solution: The Interplay Between Vibrational Relaxation, Coherence, and Solvent Effects

By using a newly implemented QM/MM multiscale MD method to simulate the excited state dynamics of the Ir2(dimen)42+ (dimen = 1,8-diisocyano-p-menthane) complex, we not only report on results that support the two experimentally observed coherent dynamical modes in the molecule but also reveal a third mode, not distinguishable by spectroscopic methods. We directly follow the channels of energy dissipation to the solvent and report that the main cause for coherence decay is the initial wide range of configurations in the excited state population. We observe that the solvent can actually extend the coherence lifetime by blocking channels for intramolecular vibrational energy redistribution (IVR).

General information
State: Published
Organisations: Center for Atomic-scale Materials Design, Department of Chemistry, Physical and Biophysical Chemistry, Department of Physics, NanoChemistry, Neutrons and X-rays for Materials Physics
Contributors: Dohn, A. O., Jónsson, E. Ö., Kjær, K. S., Brandt van Driel, T., Nielsen, M. M., Jacobsen, K. W., Henriksen, N. E., Möller, K. B.
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Web of Science (2017): Impact factor 8.709
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Scopus rating (2016): CiteScore 8.18 SJR 4.602 SNIP 1.651
Web of Science (2016): Indexed yes
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 7 SJR 3.725 SNIP 1.71
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Scopus rating (2013): CiteScore 6.61 SJR 3.529 SNIP 1.608
Web of Science (2013): Impact factor 6.687
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 6.3 SJR 3.965 SNIP 1.742
Graphene Edges Dictate the Morphology of Nanoparticles during Catalytic Channeling

We perform in-situ transmission electron microscopy (TEM) experiments of silver nanoparticles channeling on mono-, bi-, and few-layer graphene and discover that the interactions in the one-dimensional particle–graphene contact line are sufficiently strong so as to dictate the three-dimensional shape of the nanoparticles. We find a characteristic faceted shape in particles channeling along graphene 100 directions that is lost during turning and thus represents a dynamic equilibrium state of the graphene–particle system. We propose a model for the mechanism of zigzag edge formation and an explanation of the rate-limiting step for this process, supported by density functional theory (DFT) calculations, and obtain a good agreement between the DFT-predicted and experimentally obtained activation energies of 0.39 and 0.56 eV, respectively. Understanding the origin of the channels’ orientation and the strong influence of the graphene lattice on the dynamic behavior of the particle morphology could be crucial for obtaining deterministic nanopatterning on the atomic scale.

General information
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Organisations: Department of Micro- and Nanotechnology, Nanointegration, Department of Physics, Theoretical Atomic-scale Physics, Center for Electron Nanoscopy, Center for Atomic-scale Materials Design, Center for Nanostructured Graphene
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mBEEF: An accurate semi-local Bayesian error estimation density functional
We present a general-purpose meta-generalized gradient approximation (MGGA) exchange-correlation functional generated within the Bayesian error estimation functional framework [J. Wellendorff, K. T. Lundgaard, A. Mogelhøj, V. Petzold, D. D. Landis, J. K. Nørskov, T. Bligaard, and K. W. Jacobsen, Phys. Rev. B 85, 235149 (2012)]. The functional is designed to give reasonably accurate density functional theory (DFT) predictions of a broad range of properties in materials physics and chemistry, while exhibiting a high degree of transferability. Particularly, it improves upon solid cohesive energies and lattice constants over the BEEF-vdW functional without compromising high performance on adsorption and reaction energies. We thus expect it to be particularly well-suited for studies in surface science and catalysis. An ensemble of functionals for error estimation in DFT is an intrinsic feature of exchange-correlation models designed this way, and we show how the Bayesian ensemble may provide a systematic analysis of the reliability of DFT based simulations. (C) 2014 AIP Publishing LLC.

General information
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Organisations: Center for Atomic-scale Materials Design, Department of Physics, Stanford University
Contributors: Wellendorff, J., Lundgård, K. T., Jacobsen, K. W., Bligaard, T.
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Web of Science (2017): Indexed yes
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Scopus rating (2015): CiteScore 1.98 SJR 1.255 SNIP 0.964
Web of Science (2015): Impact factor 2.894
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.54 SJR 1.446 SNIP 1.02
Web of Science (2014): Impact factor 2.952
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.95 SJR 1.559 SNIP 1.174
Web of Science (2013): Impact factor 3.122
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.86 SJR 1.832 SNIP 1.137
Web of Science (2012): Impact factor 3.164
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.07 SJR 1.845 SNIP 1.215
Web of Science (2011): Impact factor 3.333
New Light-Harvesting Materials Using Accurate and Efficient Bandgap Calculations

Electronic bandgap calculations are presented for 2400 experimentally known materials from the Materials Project database and the bandgaps, obtained with different types of functionals within density functional theory and (partial) self-consistent GW approximation, are compared for 20 randomly chosen compounds forming an unconventional set of ternary and quaternary materials. It is shown that the computationally cheap GLLB-SC potential gives results in good agreement (around 15%) with the more advanced and demanding eigenvalue-self-consistent GW. This allows for a high-throughput screening of materials for different applications where the bandgaps are used as descriptors for the efficiency of a photoelectrochemical device. Here, new light harvesting materials are proposed to be used in a one-photon photoelectrochemical device for water splitting by combining the estimation of the bandgaps with the stability analysis using Pourbaix diagrams and with the evaluation of the position of the band edges. Using this methodology, 25 candidate materials are obtained and 5 of them appear to have a realistic possibility of being used as photocatalyst in a one-photon water splitting device. © 2014 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.
Plasmons on the edge of MoS₂ nanostructures

Using ab initio calculations we predict the existence of one-dimensional (1D), atomically confined plasmons at the edges of a zigzag MoS₂ nanoribbon. The strongest plasmon originates from a metallic edge state localized on the sulfur dimers decorating the Mo edge of the ribbon. A detailed analysis of the dielectric function reveals that the observed deviations from the ideal 1D plasmon behavior result from single-particle transitions between the metallic edge state and the valence and conduction bands of the MoS₂ sheet. The Mo and S edges of the ribbon are clearly distinguishable in calculated spatially resolved electron energy loss spectrum owing to the different plasmonic properties of the two edges. The edge plasmons could potentially be utilized for tuning the photocatalytic activity of MoS₂ nanoparticles.

General information
State: Published
Bandgap Engineering of Double Perovskites for One- and Two-photon Water Splitting

Computational screening is becoming increasingly useful in the search for new materials. We are interested in the design of new semiconductors to be used for light harvesting in a photoelectrochemical cell. In the present paper, we study the double perovskite structures obtained by combining 46 stable cubic perovskites which was found to have a finite bandgap in a previous screening-study. The four-metal double perovskite space is too large to be investigated completely. For this reason we propose a method for combining different metals to obtain a desired bandgap. We derive some bandgap design rules on how to combine two cubic perovskites to generate a new combination with a larger or smaller bandgap compared with the constituent structures. Those rules are based on the type of orbitals involved in the conduction bands and on the size of the two cubic bandgaps. We also see that a change in the volume has an effect on the size of the bandgap. In addition, we suggest some new candidate materials that can be used as photocatalysts in one- and two-photon water splitting devices.

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Organisations: Department of Physics, Theoretical Atomic-scale Physics
Contributors: Castelli, I. E., Thygesen, K. S., Jacobsen, K. W.
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.13 SJR 0.141 SNIP 0.089
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 0.09 SJR 0.146 SNIP 0.098
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 0.1 SJR 0.149 SNIP 0.106
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 0.07 SJR 0.146 SNIP 0.103
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 0.07 SJR 0.155 SNIP 0.121
Computational Approach to Electron Charge Transfer Reactions

The step from ab initio atomic and molecular properties to thermodynamic - or macroscopic - properties requires the combination of several theoretical tools. This dissertation presents constant temperature molecular dynamics with bond length constraints, a hybrid quantum mechanics-molecular mechanics scheme, and tools to analyse statistical data and generate relative free energies and free energy surfaces. The methodology is applied to several charge transfer species and reactions in chemical environments - chemical in the sense that solvent, counter ions and substrate surfaces are taken in to account - which directly influence the reactants and resulting reaction through both physical and chemical interactions. All methods are though general and can be applied to different types of chemistry. First, the basis of the various theoretical tools is presented and applied to several test systems to show general (or expected) properties. Properties such as in the physical and (semi-)chemical interface between classical and quantum systems and the effects of molecular bond length constraints on the temperature during simulations. As a second step the methodology is applied to the symmetric and asymmetric charge transfer reactions between several first-row transition metals in water. The results are compared to experiments and rationalised with classical analytic expressions. Shortcomings of the methods are accounted for with clear steps towards improved accuracy. Later the analysis is extended to more complex systems composed of a larger osmium complex in solution and at the solute-substrate interfaces, where in particular the redox state of the complex is controlled through chemical means. The efficiency of the hybrid-classical and quantum mechanics method is used to generate adequate statistics and a simple post-sampling scheme used to generate free energy surfaces - which compare to full ab initio calculations. In the last part both the molecular dynamics and hybrid classical and quantum mechanics method are used to generate a vast data set for the accurate analysis of dynamical structure modes. This is for a large iridium-iridium dimer complex which shows a dramatic structural (and vibrational) change upon electronic excitation.

General information
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Organisations: Center for Atomic-scale Materials Design, Department of Physics, Department of Chemistry, NanoChemistry
Contributors: Jónsson, E. Ö., Jacobsen, K. W., Thygesen, K. S., Ulstrup, J.
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Publication information
Computational Screening of Materials for Water Splitting Applications

Design new materials for energy production in a photoelectrochemical cell, where water is split into hydrogen and oxygen by solar light, is one possible solution to the problem of increasing energy demand and storage. A screening procedure based on ab-initio density functional theory calculations has been applied to guide the search for new materials. The main descriptors of the properties relevant for the screening are: heat of formation, electronic bandgap, and positions of the band edges with respect to the red-ox levels of water. A recently implemented exchange-correlation functional, called GLLB-SC, has been used for the estimation of the bandgaps. Firstly, a screening procedure has been applied to 19000 cubic perovskite structures. These are obtained by combining 52 metals together with oxygen, nitrogen, sulfur and fluorine as anions. 32 promising materials have been found for visible light harvesting, 20 for the one-photon and 12 for the two-photon water splitting process. In addition, 16 candidates were suggested for the transparent shielding of the photocatalyst. The problem of corrosion has been addressed for the candidates for the one-photon scheme using Pourbaix diagrams.

Later on, the screening has been extended to more complex structures, like double and layered perovskites and new compounds of interest for the light harvesting problem were found. In addition, the trends in the bandgaps have been studied. The bandgaps can be tuned by an opportune combination of the metal atoms in the B-ion position in the double perovskite, and of the B-metal ion with the thickness of the octahedra in the layered perovskite structure. In the first part, the crystal structure has been kept fixed. Later, the calculations were done using the structures provided by the Materials Project database, which is based on the experimental ICSD database, and the bandgaps were calculated with focus on finding materials with potential as light harvesters. 24 materials have been proposed for the one-photon water splitting and 23 for the two-photon mechanism. Another method to obtain energy from Sun is using a photovoltaic cell that converts solar light into electricity. The absorption spectra of 70 experimentally known compounds, that are expected to be useful for light-to-electricity generation, have been calculated. 17 materials have been predicted to be promising for a single-layer solar cell and 11 for a double-layer device.
Direct measurement and modulation of single-molecule coordinative bonding forces in a transition metal complex.

Coordination chemistry has been a consistently active branch of chemistry since Werner's seminal theory of coordination compounds inaugurated in 1893, with the central focus on transition metal complexes. However, control and measurement of metal-ligand interactions at the single-molecule level remain a daunting challenge. Here we demonstrate an interdisciplinary and systematic approach that enables measurement and modulation of the coordinative bonding forces in a transition metal complex. Terpyridine is derived with a thiol linker, facilitating covalent attachment of this ligand on both gold substrate surfaces and gold-coated atomic force microscopy tips. The coordination and bond breaking between terpyridine and osmium are followed in situ by electrochemically controlled atomic force microscopy at the single-molecule level. The redox state of the central metal atom is found to have a significant impact on the metal-ligand interactions. The present approach represents a major advancement in unravelling the nature of metal-ligand interactions and could have broad implications in coordination chemistry.

General information
State: Published
Organisations: NanoChemistry, Department of Chemistry, Department of Physics, Theoretical Atomic-scale Physics, Chalmers University of Technology, Chinese Academy of Sciences
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Peer-reviewed: Yes
Electrochemical CO2 and CO reduction on metal-functionalized porphyrin-like graphene

Porphyrin-like metal-functionalized graphene structures have been investigated as possible catalysts for CO2 and CO reduction to methane or methanol. The late transition metals (Cu, Ag, Au, Ni, Pd, Pt, Co, Rh, Ir, Fe, Ru, Os) and some p (B, Al, Ga) and s (Mg) metals comprised the center of the porphyrin ring. A clear difference in catalytic properties compared to extended metal surfaces was observed owing to a different electronic nature of the active site. The preference to bind hydrogen, however, becomes a major obstacle in the reaction path. A possible solution to this problem is to reduce CO instead of CO2. Volcano plots were constructed on the basis of scaling relations of reaction intermediates, and from these plots the reaction steps with the highest overpotentials were deduced. The Rh-porphyrin-like functionalized graphene was identified as the most active catalyst for producing methanol from CO, featuring an overpotential of 0.22 V. Additionally, we have also examined the hydrogen evolution and oxidation reaction, and in their case, too, Rh-porphyrin turned out to be the best catalyst with an overpotential of 0.15 V. © 2013 American Chemical Society.
Performance of genetic algorithms in search for water splitting perovskites

We examine the performance of genetic algorithms (GAs) in uncovering solar water light splitters over a space of almost 19,000 perovskite materials. The entire search space was previously calculated using density functional theory to determine solutions that fulfill constraints on stability, band gap, and band edge position. Here, we test over 2500 unique GA implementations in finding these solutions to determine whether GA can avoid the need for brute force search, and thereby enable larger chemical spaces to be screened within a given computational budget. We find that the best GAs tested offer almost a 6 times efficiency gain over random search, and are comparable to the performance of a search based on informed chemical rules. In addition, the GA is almost 10 times as efficient as random search in finding half the solutions within the search space. By employing chemical rules, the performance of the GA can be further improved to approximately 12–17 better than random search. We discuss the effect of population size, selection function, crossover function, mutation rate, fitness function, and elitism on the final result, finding that selection function and elitism are especially important to GA performance. In addition, we determine that parameters that perform well in finding solar water splitters can also be applied to discovering transparent photocorrosion shields. Our results indicate that coupling GAs to high-throughput density functional calculations presents a promising method to rapidly search large chemical spaces for technological materials.
Stability and bandgaps of layered perovskites for one- and two-photon water splitting

Direct production of hydrogen from water and sunlight requires stable and abundantly available semiconductors with well positioned band edges relative to the water red-ox potentials. We have used density functional theory (DFT) calculations to investigate 300 oxides and oxynitrides in the Ruddlesden–Popper phase of the layered perovskite structure. Based on screening criteria for the stability, bandgaps and band edge positions, we suggest 20 new materials for the light harvesting photo-electrode of a one-photon water splitting device and 5 anode materials for a two-photon device with silicon as photo-cathode. In addition, we explore a simple rule relating the bandgap of the perovskite to the number of octahedra in the layered structure and the B-metal ion. Finally, the quality of the GLLB-SC potential used to obtain the bandgaps, including the derivative discontinuity, is validated against G0W0@LDA gaps for 20 previously identified oxides and oxynitrides in the cubic perovskite structure.

General information
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Organisations: Department of Physics, Theoretical Atomic-scale Physics
Contributors: Castelli, I. E., García Lastra, J. M., Hüser, F., Thygesen, K. S., Jacobsen, K. W.
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Scopus rating (2017): CiteScore 3.28 SJR 1.653 SNIP 1.102
Web of Science (2017): Impact factor 3.579
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.97 SJR 2.183 SNIP 1.173
Web of Science (2016): Impact factor 3.786
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 2.8 SJR 2.33 SNIP 1.157
Web of Science (2015): Impact factor 3.57
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.89 SJR 2.917 SNIP 1.335
Web of Science (2014): Impact factor 3.558
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.77 SJR 2.87 SNIP 1.352
Web of Science (2013): Impact factor 3.671
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.4 SJR 3.368 SNIP 1.517
Web of Science (2012): Impact factor 4.063
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.99 SJR 3.489 SNIP 1.626
Web of Science (2011): Impact factor 4.177
Ab initio nonequilibrium quantum transport and forces with the real-space projector augmented wave method

We present an efficient implementation of a nonequilibrium Green's function method for self-consistent calculations of electron transport and forces in nanostructured materials. The electronic structure is described at the level of density functional theory using the projector augmented wave method to describe the ionic cores and an atomic orbital basis set for the valence electrons. External bias and gate voltages are treated in a self-consistent manner and the Poisson equation with appropriate boundary conditions is solved in real space. Contour integration of the Green's function and parallelization over k points and real space makes the code highly efficient and applicable to systems containing several hundreds of atoms. The method is applied to a number of different systems, demonstrating the effects of bias and gate voltages, multiterminal setups, nonequilibrium forces, and spin transport.

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Contributors: Chen, J., Thygesen, K. S., Jacobsen, K. W.
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Peer-reviewed: Yes
Computational screening of perovskite metal oxides for optimal solar light capture

One of the possible solutions to the world's rapidly increasing energy demand is the development of new photoelectrochemical cells with improved light absorption. This requires development of semiconductor materials which have appropriate bandgaps to absorb a large part of the solar spectrum at the same time as being stable in aqueous environments. Here we demonstrate an efficient, computational screening of relevant oxide and oxynitride materials based on electronic structure calculations resulting in the reduction of a vast space of 5400 different materials to only 15 promising candidates. The screening is based on an efficient and reliable way of calculating semiconductor band gaps. The outcome of the screening includes all already known successful materials of the types investigated plus some new ones which warrant further experimental investigation.
Construction of New Electronic Density Functionals with Error Estimation Through Fitting

We investigate the possibilities and limitations for the development of new electronic density functionals through large-scale fitting to databases of binding energies obtained experimentally or through high-quality calculations. We show that databases with up to a few hundred entries allow for up to the order ten parameters to be adjusted in the exchange enhancement factor. The transferability of models between data is analyzed, and it is shown to be difficult to transfer a model trained exclusively on molecular atomization energies to the treatment of chemisorption systems.

General information

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Contributors: Petzold, V., Bligaard, T., Jacobsen, K. W.
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Web of Science (2017): Impact factor 2.439
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.55 SJR 0.975 SNIP 0.877
Web of Science (2016): Impact factor 2.486
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.41 SJR 0.926 SNIP 0.777
Web of Science (2015): Impact factor 2.355
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Conventional and acoustic surface plasmons on noble metal surfaces: a time-dependent density functional theory study

First-principles calculations of the conventional and acoustic surface plasmons (CSPs and ASPs) on the (111) surfaces of Cu, Ag, and Au are presented. The effect of s-d interband transitions on both types of plasmons is investigated by comparing results from the local density approximation and an orbital-dependent exchange-correlation (xc) potential that improves the position and width of the d bands. The plasmon dispersions calculated with the latter xc potential agree well
with electron energy loss spectroscopy (EELS) experiments. For both the CSP and ASP, the same trend of Cu < Au < Ag is found for the plasmon energies and is attributed to the reduced screening by interband transitions from Cu, to Au and Ag. This trend for the ASP, however, contradicts a previous model prediction. While the ASP is seen as a weak feature in the EELS, it can be clearly identified in the static and dynamic dielectric band structure.
Density functionals for surface science: Exchange-correlation model development with Bayesian error estimation

A methodology for semiempirical density functional optimization, using regularization and cross-validation methods from machine learning, is developed. We demonstrate that such methods enable well-behaved exchange-correlation approximations in very flexible model spaces, thus avoiding the overfitting found when standard least-squares methods are applied to high-order polynomial expansions. A general-purpose density functional for surface science and catalysis studies should accurately describe bond breaking and formation in chemistry, solid state physics, and surface chemistry, and should preferably also include van der Waals dispersion interactions. Such a functional necessarily compromises between describing fundamentally different types of interactions, making transferability of the density functional approximation a key issue. We investigate this trade-off between describing the energetics of intramolecular and intermolecular, bulk solid, and surface chemical bonding, and the developed optimization method explicitly handles making the compromise based on the directions in model space favored by different materials properties. The approach is applied to designing the Bayesian error estimation functional with van der Waals correlation (BEEF-vdW), a semilocal approximation with an additional nonlocal correlation term. Furthermore, an ensemble of functionals around BEEF-vdW comes out naturally, offering an estimate of the computational error. An extensive assessment on a range of data sets validates the applicability of BEEF-vdW to studies in chemistry and condensed matter physics. Applications of the approximation and its Bayesian ensemble error estimate to two intricate surface science problems support this.
Inclusion of Dispersion Effects in Density Functional Theory: Development and Application

In this thesis, applications and development will be presented within the field of van der Waals interactions in density functional theory. The thesis is based on the three projects: i) van der Waals interactions effect on the structure of liquid water at ambient conditions, ii) development and benchmarking of a new van der Waals density functional, and iii) the application of the newly developed functional to CO desorption from Ru(0001).

The effect of van der Waals interactions in water was studied by performing ab initio molecular dynamics simulations using PBE and the two recent van der Waals density functionals optPBE-vdW and vdW-DF2 with identical computational setup. The two van der Waals functionals have been found to give excellent descriptions of the constituents of water (e.g., water dimers and hexamers). Including van der Waals interactions gives a softer water structure as seen from structural parameters and a distribution of water networks with fewer H-bonds for the van der Waals molecular dynamics simulations compared to the PBE results. The most significant change for the van der Waals molecular dynamics simulations is the oxygen-oxygen pair-correlation function, which has a much lower first peak consistent with recent experiments, while the outer structure is completely smeared out. The water structures obtained from the ab initio van der Waals simulations clearly resemble high-density liquid water, whereas the PBE molecular dynamics simulation with equivalent computational setup resembles low-density liquid. Mixing the vdW-DF2 and the experimental low-density liquid in a 70/30% ratio gives agreement with experimental results. This is consistent with the bimodal picture of water.

Also, in this thesis the BEEF-vdW exchange-correlation functional is presented based on fitting to high-level ab initio and experimental results. The fitting scheme, based on Bayesian theory, focuses on the three aspects: a) model space, b) datasets, and c) model selection. The model space consists of a flexible expansion of the exchange enhancement factor in the generalized gradient approximation plus local density approximation, and the non-local Rutgers-Chalmers correlations. The datasets are chosen to represent gas phase chemistry, surface chemistry, solid state physics, and non-covalently bound systems in order to produce a generally applicable functional that is particularly useful for catalysis. The model selection is a two-step scheme. First the model is fitted to the individual datasets, and subsequently the combined solution are found. To avoid overfitting, a regularization term is added to the cost function, which punishes non-smooth functions and effectively reduces the 31 parameters to close to 7. The ideal weights for the combined solution are found by minimizing the product of relative cost functions. Error estimation is naturally obtained from a distribution of functionals around the optimum solution. The produced exchange-correlation functional is benchmarked against various other exchange-correlation functionals, and is seen to indeed be generally applicable, contrary to other fitted van der Waals functionals.

Lastly, the newly developed BEEF-vdW exchange-correlation functional is applied to the desorption of CO from Ru(0001). The results here support and help interpret the very first spectroscopic measurement of a precursor state performed as a pump-probe experiment at the Linac Coherent Light Source at Stanford Linear Accelerator Center. The support from the theoretical point of view is based on the potential of mean force, which is a free energy potential curve where all degrees of freedom except the reaction coordinate have been thermally averaged. The potential of mean force develops an adsorption/desorption barrier for increasing temperatures and a second minimum occurs at larger surface separations. A correct description of both the chemical interaction and the long-range van der Waals interactions is essential to describe the adsorption/desorption process and commonly used generalized gradient approximation functionals are seen to be incapable of this.

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Investigation of Catalytic Finite-Size-Effects of Platinum Metal Clusters

In this paper, we use density functional theory (DFT) calculations on highly parallel computing resources to study size-dependent changes in the chemical and electronic properties of platinum (Pt) for a number of fixed freestanding clusters ranging from 13 to 1415 atoms, or 0.7–3.5 nm in diameter. We find that the surface catalytic properties of the clusters converge to the single crystal limit for clusters with as few as 147 atoms (1.6 nm). Recently published results for gold (Au) clusters showed analogous convergence with size. However, this convergence happened at larger sizes, because the Au d-states do not contribute to the density of states around the Fermi-level, and the observed level fluctuations were not significantly damped until the cluster reached ca. 560 atoms (2.7 nm) in size.

General information
New cubic perovskites for one- and two-photon water splitting using the computational materials repository

A new efficient photoelectrochemical cell (PEC) is one of the possible solutions to the energy and climate problems of our time. Such a device requires development of new semiconducting materials with tailored properties with respect to stability and light absorption. Here we perform computational screening of around 19,000 oxides, oxynitrides, oxysulfides, oxyfluorides, and oxyfluoronitriles in the cubic perovskite structure with PEC applications in mind. We address three main applications: light absorbers for one- and two-photon water splitting and high-stability transparent shields to protect against corrosion. We end up with 20, 12, and 15 different combinations of oxides, oxynitrides and oxyfluorides, respectively, inviting further experimental investigation.

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Organisations: Department of Physics, Theoretical Atomic-scale Physics, Center for Atomic-scale Materials Design, Experimental Surface and Nanomaterials Physics, Center for Individual Nanoparticle Functionality, Stanford University
Contributors: Castelli, I. E., Landis, D., Thygesen, K. S., Dahl, S., Chorkendorff, I., Jaramillo, T. F., Jacobsen, K. W.
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Optical properties of bulk semiconductors and graphene/boron nitride: the Bethe-Salpeter equation with derivative discontinuity-corrected density functional energies

We present an efficient implementation of the Bethe-Salpeter equation (BSE) for optical properties of materials in the projector augmented wave method Grid-based projector-augmented wave method (GPAW). Single-particle energies and wave functions are obtained from the Gritsenko, Leeuwen, Lenthe, and Baerends potential [Phys. Rev. A51, 1944 (1995)] with the modifications from Kuisma et al. [Phys. Rev. B82, 115106 (2010)] GLLBSC functional which explicitly includes the derivative discontinuity, is computationally inexpensive, and yields excellent fundamental gaps. Electron-hole interactions are included through the BSE using the statically screened interaction evaluated in the random phase approximation. For a representative set of semiconductors and insulators we find excellent agreement with experiments for the dielectric functions, onset of absorption, and lowest excitonic features. For the two-dimensional systems of graphene and hexagonal boron-nitride (h-BN) we find good agreement with previous many-body calculations. For the graphene/h-BN interface we find that the fundamental and optical gaps of the h-BN layer are reduced by 2.0 and 0.7 eV, respectively, compared to freestanding h-BN. This reduction is due to image charge screening which shows up in the GLLBSC calculation as a reduction (vanishing) of the derivative discontinuity.

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Oxidative trends of TiO$_2$—hole trapping at anatase and rutile surfaces

Understanding the nature of photogenerated carriers in a photocatalyst is central to understanding its photocatalytic performance. Based on density functional theory calculation we show that for TiO$_2$, the most popular photo-catalyst, the electron hole self-trapping leads to band gap states which position is dependent on the type of surface termination. Such variations in hole state energies can lead to differences in photocatalytic activity among rutile and anatase surface facets. We find that the calculated hole state energies correlate with photo-deposition and photo-etching rates. We anticipated that our results can aid the design of more reactive photo-catalysts based on TiO$_2$ and our approach can be utilized for other relevant photo-catalysts as well.
Phonon-limited mobility in n-type single-layer MoS2 from first principles

We study the phonon-limited mobility in intrinsic n-type single-layer MoS2 for temperatures T > 100 K. The materials properties including the electron-phonon interaction are calculated from first principles and the deformation potentials and Frohlich interaction in single-layer MoS2 are established. The calculated room-temperature mobility of similar to 410 cm²V⁻¹s⁻¹ is found to be dominated by optical phonon scattering via intra and intervalley deformation potential couplings and the Frohlich interaction. The mobility is weakly dependent on the carrier density and follows a μ similar to T-γ temperature dependence with γ = 1.69 at room temperature. It is shown that a quenching of the characteristic homopolar mode, which is likely to occur in top-gated samples, increases the mobility with similar to 70 cm²V⁻¹s⁻¹ and can be observed as a decrease in the exponent to γ = 1.52. In comparison to recent experimental findings for the mobility in single-layer MoS2 (similar to 200 cm²V⁻¹s⁻¹), our results indicate that mobilities close to the intrinsic phonon-limited mobility can be achieved in two-dimensional materials via dielectric engineering that effectively screens static Coulomb scattering on, e.g., charged impurities.

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Scanning Tunneling Microscopy Evidence for the Dissociation of Carbon Monoxide on Ruthenium Steps

In heterogeneous catalysis, identifying the active site for key reaction steps is an important contribution for the optimization of industrial synthesis. The structure sensitivity of CO dissociation on a metal catalyst, which is the rate-limiting step for the methanation and the Fischer–Tropsch processes under certain conditions, has been debated for years. Here, scanning tunneling microscopy (STM) and density functional theory (DFT) are used to clarify the role of monatomic steps in the splitting of CO on a stepped Ru(0 1 54) crystal, which displays alternating steps with either 4-fold or 3-fold symmetry. After CO doses at elevated temperatures, the STM images reveal step decorations characteristic of atomic oxygen resulting from CO dissociation on every second step. The comparison of the STM images with the results of DFT calculations shows that the step decoration occurs on the steps displaying the 4-fold symmetry. We conclude that the active sites for CO dissociation on ruthenium are located on the 4-fold symmetry monatomic steps.
Spatially resolved quantum plasmon modes in metallic nano-films from first-principles

Electron energy loss spectroscopy (EELS) can be used to probe plasmon excitations in nanostructured materials with atomic-scale spatial resolution. For structures smaller than a few nanometers, quantum effects are expected to be important, limiting the validity of widely used semiclassical response models. Here we present a method to identify and compute spatially resolved plasmon modes from first-principles based on a spectral analysis of the dynamical dielectric function. As an example we calculate the plasmon modes of 0.5 to 4 nm thick Na films and find that they can be classified as (conventional) surface modes, subsurface modes, and a discrete set of bulk modes resembling standing waves across the film. We find clear effects of both quantum confinement and nonlocal response. The quantum plasmon modes provide an intuitive picture of collective excitations of confined electron systems and offer a clear interpretation of spatially resolved EELS spectra.
The Computational Materials Repository
The possibilities for designing new materials based on quantum physics calculations are rapidly growing, but these design efforts lead to a significant increase in the amount of computational data created. The Computational Materials Repository (CMR) addresses this data challenge and provides a software infrastructure that supports the collection, storage, retrieval, analysis, and sharing of data produced by many electronic-structure simulators.

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Organisations: Department of Physics, Theoretical Atomic-scale Physics, Stanford University, Argonne National Laboratory, University of Chicago
Unraveling the acoustic electron-phonon interaction in graphene

Using a first-principles approach we calculate the electron-phonon couplings in graphene for the transverse and longitudinal acoustic phonons. Analytic forms of the coupling matrix elements valid in the long-wavelength limit are found to give an almost quantitative description of the first-principles matrix elements even at shorter wavelengths. Using the analytic forms of the coupling matrix elements, we study the acoustic phonon-limited carrier mobility and quasiparticle lifetime observable in photoemission spectroscopy for temperatures 0-200 K and high carrier densities of 10^{12}-10^{13} cm^{-2}. We find that the intrinsic effective acoustic deformation potential of graphene is Ξ_{eff}=6.8 eV and that the temperature dependence of the mobility μ~T^{-α} in the Bloch-Grüneisen regime increases beyond an α=4 dependence even in the absence of screening when the true coupling matrix elements are considered. The α>4 temperature dependence of the mobility is found to originate in a similar temperature dependence of the relaxation time at the Fermi level. The large disagreement between our calculated deformation potential and those extracted from experimental measurements (18-29 eV) indicates that additional or modified acoustic phonon-scattering mechanisms are at play in experimental situations.

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Versatile Density Functionals for Computational Surface Science

Density functional theory (DFT) emerged almost 50 years ago. Since then DFT has established itself as the central electronic structure methodology for simulating atomicscale systems from a few atoms to a few hundred atoms. This success of DFT is due to a very favorable accuracy-to-computational cost ratio. In a wide range of applications, in fields as diverse as condensed matter physics over geophysics, chemistry, and chemical engineering to molecular biology, DFT now continuously delivers the theoretical base for experimental interpretation and forms an essential component for establishing reliable insights and generation of knowledge. In spite of the great successes of DFT, fundamental challenges still exist for the theory. Systematic improvement of the central ingredient in the theory—the approximate exchange–correlation functional—is by no means a straightforward task: Some materials and chemical properties are simply not treated acceptably well, errors are unknown and often difficult to control, and it is difficult to evaluate whether a highly optimized, empirically fitted, functional is truly a “good” functional or whether it is merely over-parametrized and overfitted. In this thesis I address these problems systematically. It is here analyzed carefully which ingredients must be included to establish a functional which simultaneously performs well for a range of important materials and chemical properties. A general methodology is defined for the multi-objective fitting of exchange–correlation functionals in a language that naturally allows for error prediction within DFT. The optimization methodology includes as a central ingredient establishment of a compromise between high transferability (measured by the smoothness of the resulting functional) and low prediction error using statistical resampling techniques, thereby systematically avoiding problems with overfitting. The first ever density functional presenting both reliable accuracy and convincing error estimation is generated. The methodology is general enough to be applied to more complex functional forms with higher-dimensional fitting and resampling. This is illustrated by searching for meta-GGA type functionals that outperform current meta-GGAs while
Accurate treatment of nanoelectronics through improved description of van der Waals Interactions

This thesis emerges from a patented idea to utilize intentionally structured surfaces and differences in adsorption strengths to self-assemble some source material into nanoelectronic components, and ends up in the heated debate regarding structure of ambient water. It investigates the role and relevance of van der Waals (vdW) forces in molecular surface adsorption and water through density-functional theory (DFT), using the exchange-correlation functional vdW-DF [Dion et al., Phys. Rev. Lett. 92, 246401 (2004)] and developments based on it. Results are first computed for adsorption with vdW forces of, e.g., benzene on Au(111) and other coinage metals, phenol on nickel, and graphene on Co, Ni, Pd, Ag, Au, Cu and Pt surfaces. The vdW forces are ubiquitous but for transition metals and on structured surfaces, with defects, incl. The vdW adsorbate attraction benefits from the two-dimensional extent of the surface and favors adsorption sites close to the surface, while the Pauli repulsion keeps the adsorbate away. Impurities, like an adatom or an adsorbed pyramid, pushes the adsorbate away from surface, giving a reduction of the attraction due to vdW forces. In this way the vdW force varies on an atomic scale, and in the weak-adsorption limit coordination rules for adsorption are affected. The thesis illustrates this force competition by varying adsorption site and substrate to find examples where the rule of undercoordination which holds according to DFT without vdW forces, does not when accounting for vdW. An evaluation of the vdW-DF method is made by comparison with a detailed experimentally determined physisorption-potential for H2 on Cu(111). The vdW-DF potential-energy curves appear to have an agreement at large with the measured curve.

Competition between different kinds of forces rules also other systems. For instance, in water complexes hydrogen bonds compete with vdW force, just like chemisorptive forces due to d-electrons do on transition metals. Bond lengths are shorter than those for typical vdW bonds also here, making both adsorption and water call for improved exchange functionals. DFT calculations are performed for water dimer and hexamer, and for liquid water. Calculations on four low-energetic isomers of the water hexamer show that the vdW-DF accurately determines the energetic trend on these small clusters. However, the dissociation-energy values with the vdW-DF functional are too small, as the exchange approximation used is too repulsive. With the vdW-DF and other functionals that account for vdW forces, the total isomer energies are minimized in molecular configurations, which are compact, and in which many hydrogen bonds (HBs) can be described as distorted, or even as broken. The hexamer experience of the criteria and effects of vdW forces can be used in interpretation of results of molecular dynamics (MD) simulations of ambient water, where vdW forces qualitatively result in liquid water with fewer, more distorted HBs. This is interesting as there is currently a heated debate in the water community on the level of HB distortion in ambient water, and where MD simulations without first principles vdW forces have played an important role to suggest that liquid water is almost tetrahedral, with few distorted HBs. Simulations with improved vdW-DF functionals, called vdW-DF2 and opIPBE-vdW, result in a structure similar to the HDL phase (high-density liquid) under proper conditions, and thus show thatvdW forces may be vital in the two-liquid model suggested in http://www.sciencemag.org/content/304/5673/995.abstract.
Ab Initio Calculations of the Electronic Properties of Polypyridine Transition Metal Complexes and Their Adsorption on Metal Surfaces in the Presence of Solvent and Counterions

Os(II)/(III) and Co(II)/(III) polypyridine complexes in aqueous solution are robust molecular entities both in freely solute state and adsorbed on Au(111)- and Pt(111)-electrode surfaces. This class of robust coordination chemical compounds have recently been characterized by electrochemical scanning tunneling microscopy (in situ STM). The Os-complexes were found to display strong tunneling spectroscopic (STS) features at the level of resolution of the single molecule while STS features of the Co complexes, although clear, were much weaker. The data was framed by concise but phenomenological theory of interfacial electrochemical electron transfer extended to the electrochemical in situ STM configuration. With a view on first-principle insight into the in situ STM behavior of robust redox (as opposed to nonredox) molecules, we present in this report a density functional theory (DFT) study of the complexes in both free and adsorbate state, in either state exposed to both stoichiometric counterions and a large assembly of solvent water molecules. The oxidation states of the complexes were controlled, first by introducing chlorine counter atoms followed by spontaneous attraction of electrons from the complexes, also at first in electrostatically neutral form. Second, the solvent is found to provide strong dielectric screening of this charge transfer process and to be crucial for achieving the full chemically meaningful charge separated ionic oxidation states. The molecular charge and structure of the complexes in the presence of the solvent, are conserved upon adsorption, whereas the structural features of the different oxidation states are completely lost upon adsorption under vacuum conditions. Detailed microscopic insight such as offered by the present study will be important in molecular-based approaches to "smart" redox molecules enclosed in in situ STM or other nanoscale and single-molecules scale configurations in condensed matter environments.
Ab initio van der Waals interactions in simulations of water alter structure from mainly tetrahedral to high-density-like.

The structure of liquid water at ambient conditions is studied in ab initio molecular dynamics simulations in the NVE ensemble using van der Waals (vdW) density-functional theory, i.e., using the new exchange-correlation functionals optPBE-vdW and vdw-DF2, where the latter has softer nonlocal correlation terms. Inclusion of the more isotropic vdW interactions counteracts highly directional hydrogen bonds, which are enhanced by standard functionals. This brings about a softening of the microscopic structure of water, as seen from the broadening of angular distribution functions and, in particular, from the much lower and broader first peak in the oxygen-oxygen pair-correlation function (PCF) and loss of structure in the outer hydration shells. Inclusion of vdW interactions is shown to shift the balance of resulting structures from open tetrahedral to more close-packed. The resulting O-O PCF shows some resemblance with experiment for high-density water (Soper, A. K. and Ricci, M. A. Phys. Rev. Lett. 2000, 84, 2881), but not directly with experiment for ambient water. Considering the accuracy of the new functionals for interaction energies, we investigate whether the simulation protocol could cause the deviation. An O-O PCF consisting of a linear combination of 70% from vdw-DF2 and 30% from low-density liquid water, as extrapolated from experiments, reproduces near-quantitatively the experimental O-O
PCF for ambient water. This suggests the possibility that the new functionals may be reliable and that instead larger-scale simulations in the NPT ensemble, where the density is allowed to fluctuate in accordance with proposals for supercooled water, could resolve the apparent discrepancy with the measured PCF.
Efficient electronic structure methods applied to metal nanoparticles

Nano-scale structures are increasingly applied in the design of catalysts and electronic devices. A theoretical understanding of the basic properties of such systems is enabled through modern electronic structure methods such as density functional theory. This thesis describes the development of efficient approaches to density functional theory and the application of these methods to metal nanoparticles.

We describe the formalism and implementation of localized atom-centered basis sets within the projector augmented wave method. Basis sets allow for a dramatic increase in performance compared to plane-wave or real-space methods, but sacrifice accuracy in doing so. This approach is implemented in the GPAW code where it complements the existing real-space approach. For both the real-space and basis set methods we implement parallel code to adapt GPAW for large-scale calculations on the BlueGene/P architecture. Real-space calculations are performed to investigate the convergence of chemical properties of Au and Pt clusters toward the bulk limit. Specifically we study chemisorption of O and CO on cuboctahedral clusters up to 1415 atoms using up to 65536 CPU cores. Small clusters almost universally bind more strongly than large ones. This can be understood mostly as a geometric effect. Convergence of chemisorption energies within 0.1 eV of bulk values happens at about 200 atoms for Pt and 600 atoms for Au. Particularly for O on Au, large variations due to electronic effects are seen for smaller clusters. The basis set method is used to study the electronic effects for the contiguous range of clusters up to several hundred atoms. The s-electrons hybridize to form electronic shells consistent with the jellium model, leading to electronic magic numbers for clusters with full shells. Large electronic gaps and jumps in Fermi level near magic numbers can lead to alkali-like or halogen-like behaviour when main-group atoms adsorb onto gold clusters. A non-self-consistent NewnsAnderson model is used to more closely study the chemisorption of main-group atoms on magic-number Au clusters. The behaviour at magic numbers can be understood from the location of adsorbateinduced states relative to the Fermi level. The relationship between geometric and electronic effects in Au is studied by rough first-principles simulated annealings with up to 150 atoms. Non-magic clusters are found to deform considerably, reducing the total energy through the creation of gaps. Clusters larger than 100 atoms can elongate systematically by up to 15%. This demonstrates a complex interdependence between electronic and geometric structure in a size regime which in most cases has been studied semiempirically.
Electronic hole localization in rutile and anatase TiO2 - Self-interaction correction in Δ-Self-Consistent Field Density Functional Theory

We study electronic hole localization in rutile and anatase titanium dioxide by means of Δ-Self-Consistent Field Density Functional Theory. In order to compare stabilities of the localized and the delocalized hole states we introduce a simple correction to the wrong description of the localization processes within DFT. The correction removes the non-linearity of energy for fractional excitations. We show that the self-trapped and the delocalized hole states have comparable stability in rutile TiO2 whereas in anatase the former is favoured. The theoretical prediction of the adiabatic Potential Energy Surfaces for the hole localization compares well with published photoluminescence measurements.
Electronic hole transfer in rutile and anatase TiO₂: Effect of a delocalization error in the density functional theory on the charge transfer barrier height

We analyze the deformation of the potential energy surface (PES) due to the incorrect description of fractional electron systems (the nonlinearity of the energy with electron number) within a (semi) local density functional theory (DFT). Particularly sensitive to this failure are polaronic systems where charge localization is strongly coupled to lattice distortion. As an example we calculate the adiabatic PES for the hole transfer process in rutile and anatase TiO₂. (Semi) local DFT leads to qualitatively wrong, barrierless curves. Removal of the nonlinearity improves the PES shape and allows us to calculate hole mobilities.

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Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 2.789 SNIP 1.541
We use density functional theory (DFT) to investigate the electronic structure and chemical properties of gold nanoparticles. Different structural families of clusters are compared. For up to 60 atoms we optimize structures using DFT-based simulated annealing. Cluster geometries are found to distort considerably, creating large band gaps at the Fermi level. For up to 200 atoms we consider structures generated with a simple EMT potential and clusters based on cuboctahedra and icosahedra. All types of cluster geometry exhibit jelliumlike electronic shell structure. We calculate adsorption energies of several atoms on the cuboctahedral clusters. Adsorption energies are found to vary abruptly at magic numbers. Using a Newns-Anderson model we find that the effect of magic numbers on adsorption energy can be understood from the location of adsorbate-induced states with respect to the cluster Fermi level.
Finite Size Effects in Chemical Bonding: From Small Clusters to Solids

We address the fundamental question of which size a metallic nano-particle needs to have before its surface chemical properties can be considered to be those of a solid, rather than those of a large molecule. Calculations of adsorption energies for carbon monoxide and oxygen on a series of gold nanoparticles ranging from 13 to 1,415 atoms, or 0.8–3.7 nm, have been made possible by exploiting massively parallel computing on up to 32,768 cores on the Blue Gene/P computer at Argonne National Laboratory. We show that bulk surface properties are obtained for clusters larger than ca. 560 atoms (2.7 nm). Below that critical size, finite-size effects can be observed, and we show those to be related to variations in the local atomic structure augmented by quantum size effects for the smallest clusters.
First-principles study of surface plasmons on Ag(111) and H/Ag(111)

Linear-response time-dependent density functional theory is used to investigate the relation between molecular bonding and surface plasmons for the model system H/Ag(111). We employ an orbital-dependent exchange-correlation functional to obtain a correct description of the Ag 3d band, which is crucial to avoid overscreening the plasmon by the s-d interband transitions. For the clean surface, this approach reproduces the experimental plasmon energies and dispersion to within 0.15 eV. Adsorption of hydrogen shifts and damps the Ag(111) surface plasmon and induces a new peak in the loss function at 0.6 eV below the Ag(111) plasmon peak. This feature originates from interband transitions between states located on the hydrogen atoms and states on the Ag surface atoms.
We present an implementation of the linear density response function within the projector-augmented wave method with applications to the linear optical and dielectric properties of both solids, surfaces, and interfaces. The response function is
represented in plane waves while the single-particle eigenstates can be expanded on a real space grid or in atomic-orbital basis for increased efficiency. The exchange-correlation kernel is treated at the level of the adiabatic local density approximation (ALDA) and crystal local field effects are included. The calculated static and dynamical dielectric functions of Si, C, SiC, AIP, and GaAs compare well with previous calculations. While optical properties of semiconductors, in particular excitonic effects, are generally not well described by ALDA, we obtain excellent agreement with experiments for the surface loss function of graphene and the Mg(0001) surface with plasmon energies deviating by less than 0.2 eV. Finally, the method is applied to study the influence of substrates on the plasmon excitations in graphene.

General information
State: Published
Organisations: Theoretical Atomic-scale Physics, Department of Physics
Contributors: Yan, J., Mortensen, J. J., Jacobsen, K. W., Thygesen, K. S.
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ISSN (Print): 0163-1829
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
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Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Impact factor 3.813
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Impact factor 3.836
Web of Science (2016): Indexed yes
Scopus rating (2015): CiteScore 2.8 SJR 2.377 SNIP 1.13
Web of Science (2015): Impact factor 3.718
Web of Science (2015): Indexed yes
Scopus rating (2014): CiteScore 3.3 SJR 2.762 SNIP 1.316
Web of Science (2014): Impact factor 3.736
Web of Science (2014): Indexed yes
Scopus rating (2013): CiteScore 3.55 SJR 2.813 SNIP 1.326
Web of Science (2013): Impact factor 3.664
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): CiteScore 3.57 SJR 3.173 SNIP 1.378
Web of Science (2012): Impact factor 3.767
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): CiteScore 3.61 SJR 3.326 SNIP 1.423
Web of Science (2011): Impact factor 3.691
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 3.318 SNIP 1.447
Web of Science (2010): Impact factor 3.774
Web of Science (2010): Indexed yes
Web of Science (2009): Indexed yes
Scopus rating (2008): SJR 2.923 SNIP 1.516
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.892 SNIP 1.588
Nonlocal Screening of Plasmons in Graphene by Semiconducting and Metallic Substrates: First-Principles Calculations

We investigate the role of substrates on the collective excitations of graphene by using a first-principles implementation of the density response function within the random-phase approximation. Specifically, we consider graphene adsorbed on SiC(0001) and Al(111) as representative examples of a semiconducting and metallic substrate. On SiC(0001), the long wavelength π plasmons are significantly damped although their energies remain almost unaltered. On Al(111), the long wavelength π plasmons are completely quenched due to the coupling to the metal surface plasmon. The strong damping of the plasmon excitations occurs despite the fact that the single-particle band structure of graphene is completely unaffected by the substrates illustrating the nonlocal nature of the effect.
Semiconductor Photocatalysis: Electronic Hole Trapping in TiO₂

Photocatalysis (the acceleration of a photo-reaction in the presence of a catalyst) is presently used in large variety of applications and is one of the possible strategies for future sustainable fuel production from solar energy. A general picture of a photocatalytic process is well known: photogeneration of electron-hole pairs,
excess carrier transport to distinct reactive sites and finally carrier utilization in a chemical reaction. For most photocatalyst a detailed understanding of these steps, however, is lacking yet it is crucial to elucidate photocatalyst limitations. Of particular importance is gaining insight into the nature of photogenerated carriers as they play a central role in all the basics steps of a photocatalytic process.

The main objective of this thesis is to elucidate the experimentally observed localized nature of photogenerated electron holes in titanium dioxide—the most studied, yet poorly understood photocatalyst.

By means of the density functional theory (DFT) and its simple extension, the linear expansion self-consistent field DFT, it is shown that in TiO2 the photogenerated holes self-trap forming O− small polarons. Self-trapping strength is significantly modified in surface layers due to the variation of surface electrostatic potential. This finding explains differences in photooxidative properties among rutile and anatase TiO2 facades. Optical absorption spectra and hole hopping mobilities of the O− centers in TiO2 have been calculated. Since time resolved optical spectroscopies are common techniques to study hole dynamics in TiO2, these results should aid analysis of photocatalytic processes on TiO2.

Apart from photocatalysis this thesis also deals with the problem of the localization/delocalization error in approximate DFT functionals—the effect of the incorrect, nonlinear description of fractional electron systems by approximate exchange-correlation functionals. It is shown that by removing the total energy nonlinearity a more consistent description of states with different degrees of localization can be achieved.

General information
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Organisations: Department of Physics, Theoretical Atomic-scale Physics
Contributors: Zawadzki, P., Rossmeisl, J., Jacobsen, K. W.
Number of pages: 138
Publication date: 2011

Publication information
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Original language: English
Electronic versions:
Pawel_Zawadzki.pdf
Research output: Research › Ph.D. thesis – Annual report year: 2012

Trends in Metal Oxide Stability for Nanorods, Nanotubes, and Surfaces
The formation energies of nanostructures play an important role in determining their properties, including their catalytic activity. For the case of 15 different rutile and 8 different perovskite metal oxides, we used density functional theory (DFT) to calculate the formation energies of (2,2) nanorods, (3,3) nanotubes, and the (110) and (100) surfaces. These formation energies can be described semiquantitatively (mean absolute error = 0.12 eV) by the fraction of metal–oxygen bonds broken and the metal d-band and p-band centers in the bulk metal oxide.

General information
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Organisations: Department of Physics, Theoretical Atomic-scale Physics
Contributors: Mowbray, D., Martinez, J. I., Vallejo, F. C., Rossmeisl, J., Thygesen, K. S., Jacobsen, K. W., Nørskov, J. K.
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Publication information
Journal: Journal of Physical Chemistry Part C: Nanomaterials and Interfaces
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
Web of Science (2017): Impact factor 4.84
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Communications: Elementary oxygen electrode reactions in the aprotic Li-air battery
We discuss the electrochemical reactions at the oxygen electrode of an aprotic Li-air battery. Using density functional theory to estimate the free energy of intermediates during the discharge and charge of the battery, we introduce a reaction free energy diagram and identify possible origins of the overpotential for both processes. We also address the question of electron conductivity through the Li2O2 electrode and show that in the presence of Li vacancies Li2O2 becomes a conductor.
Computer simulations of nanoindentation in Mg-Cu and Cu-Zr metallic glasses

The formation of shear bands during plastic deformation of Cu0.50Zr0.50 and Mg0.85Cu0.15 metallic glasses is studied using atomic-scale computer simulations. The atomic interactions are described using realistic many-body potentials within the effective medium theory, and are compared with similar simulations using a Lennard-Jones description of the material. The metallic glasses are deformed both in simple shear and in a simulated nanoindentation experiment. Plastic shear localizes into shear bands with a width of approximately 5 nm in CuZr and 8 nm in MgCu. In simple shear, the shear band formation is very clear, whereas only incipient shear bands are seen in nanoindentation. The shear band formation during nanoindentation is sensitive to the indentation velocity, indenter radius and the cooling rate during the formation of the metallic glass. For comparison, a similar nanoindentation simulation was made with a nanocrystalline sample, showing how the presence of a polycrystalline structure leads to a different and more spatially distributed deformation pattern, where dislocation avalanches play an important role.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Theoretical Atomic-scale Physics, Roskilde University
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Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Modelling and Simulation in Materials Science and Engineering
Volume: 18
Issue number: 5
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Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 1.8 SJR 0.821 SNIP 0.93
Web of Science (2017): Impact factor 1.793
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 1.82 SJR 1.076 SNIP 1.05
Web of Science (2016): Impact factor 1.891
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 1.73 SJR 1.225 SNIP 1.057
Web of Science (2015): Impact factor 1.859
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 1.81 SJR 1.305 SNIP 1.157
Web of Science (2014): Impact factor 2.167
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 1.25 SJR 1.083 SNIP 1.197
Web of Science (2013): Impact factor 1.492
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.05 SJR 1.461 SNIP 1.794
Web of Science (2012): Impact factor 1.932
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 1.96 SJR 1.151 SNIP 1.362
Web of Science (2011): Impact factor 2.298
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Designing multifunctional chemical sensors using Ni and Cu doped carbon nanotubes

We demonstrate a "bottom up" approach to the computational design of a multifunctional chemical sensor. General techniques are employed for describing the adsorption coverage and resistance properties of the sensor based on density functional theory and non-equilibrium Green's function methodologies, respectively. Specifically, we show how Ni and Cu doped metallic (6,6) single-walled carbon nanotubes may work as effective multifunctional sensors for both CO and NH3.

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Organisations: Department of Physics, Theoretical Atomic-scale Physics
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Journal: IPPS physica status solidi (b)
Volume: 247
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.67 SJR 0.602 SNIP 0.786
Web of Science (2017): Impact factor 1.729
Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method

Electronic structure calculations have become an indispensable tool in many areas of materials science and quantum chemistry. Even though the Kohn-Sham formulation of the density-functional theory (DFT) simplifies the many-body problem significantly, one is still confronted with several numerical challenges. In this article we present the projector augmented-wave (PAW) method as implemented in the GPAW program package (https://wiki.fysik.dtu.dk/gpaw) using a uniform real-space grid representation of the electronic wavefunctions. Compared to more traditional plane wave or localized basis set approaches, real-space grids offer several advantages, most notably good computational scalability and systematic convergence properties. However, as a unique feature GPAW also facilitates a localized atomic-orbital basis set in addition to the grid. The efficient atomic basis set is complementary to the more accurate grid, and the possibility to seamlessly switch between the two representations provides great flexibility. While DFT allows one to study ground state properties, time-dependent density-functional theory (TDDFT) provides access to the excited states. We have implemented the two common formulations of TDDFT, namely the linear-response and the time propagation schemes. Electron transport calculations under finite-bias conditions can be performed with GPAW using non-equilibrium Green functions and the localized basis set. In addition to the basic features of the real-space PAW method, we also describe the implementation of selected exchange-correlation functionals, parallelization schemes, Delta SCF-method, x-ray absorption spectra, and maximally localized Wannier orbitals.
The stability of graphene nanoribbons in the presence of typical atmospheric molecules is systematically investigated by means of density-functional theory. We calculate the edge formation free energy of five different edge configurations passivated by H, H2, O, O2, N2, CO, CO2, and H2O, respectively. In addition to the well known hydrogen passivated armchair and zigzag edges, we find the edges saturated by oxygen atoms to be particularly stable under atmospheric conditions. Saturation of the zigzag edge by oxygen leads to the formation of metallic states strictly localized on the oxygen atoms. Finally, the vibrational spectrum of the hydrogen- and oxygen-passivated ribbons are calculated and compared.

First-principles calculations of graphene nanoribbons in gaseous environments: Structural and electronic properties

The stability of graphene nanoribbons in the presence of typical atmospheric molecules is systematically investigated by means of density-functional theory. We calculate the edge formation free energy of five different edge configurations passivated by H, H2, O, O2, N2, CO, CO2, and H2O, respectively. In addition to the well known hydrogen passivated armchair and zigzag edges, we find the edges saturated by oxygen atoms to be particularly stable under atmospheric conditions. Saturation of the zigzag edge by oxygen leads to the formation of metallic states strictly localized on the oxygen atoms. Finally, the vibrational spectrum of the hydrogen- and oxygen-passivated ribbons are calculated and compared.

General information
State: Published
Organisations: Theoretical Atomic-scale Physics, Department of Physics, Section for Structural Engineering, Department of Civil Engineering
First-principles modelling of scanning tunneling microscopy using non-equilibrium Green's functions

The investigation of electron transport processes in nano-scale architectures plays a crucial role in the development of surface chemistry and nano-technology. Experimentally, an important driving force within this research area has been the concurrent refinements of scanning tunneling microscopy (STM) techniques. The theoretical treatment of the STM operation has traditionally been based on the Bardeen and Tersoff-Hamann methods which take as input the single-particle wave functions and eigenvalues obtained from finite cluster or slabs models of the surface-tip interface. Here, we present a novel STM simulation scheme based on non-equilibrium Green's functions (NEGF) and Wannier functions which is both accurate and very efficient. The main novelty of the scheme compared to the Bardeen and Tersoff-Hamann approaches is that the coupling to the infinite (macroscopic) electrodes is taken into account. As an illustrating example we apply the NEGF-STM method to the Si(001)(2x1):H surface with sub-surface P doping and discuss the results in comparison to the Bardeen and Tersoff-Hamann methods.
Fully self-consistent GW calculations for molecules

We calculate single-particle excitation energies for a series of 34 molecules using fully self-consistent GW, one-shot G0W0, Hartree-Fock (HF), and hybrid density-functional theory (DFT). All calculations are performed within the projector-augmented wave method using a basis set of Wannier functions augmented by numerical atomic orbitals. The GW self-energy is calculated on the real frequency axis including its full frequency dependence and off-diagonal matrix elements. The mean absolute error of the ionization potential (IP) with respect to experiment is found to be 4.4, 2.6, 0.8, 0.4, and 0.5 eV for DFT-PBE, DFT-PBE0, HF, G0W0(HF), and self-consistent GW, respectively. This shows that although electronic screening is weak in molecular systems, its inclusion at the GW level reduces the error in the IP by up to 50% relative to unscreened HF. In general GW overscreens the HF energies leading to underestimation of the IPs. The best IPs are obtained from one-shot G0W0 calculations based on HF since this reduces the overscreening. Finally, we find that the inclusion of core-valence exchange is important and can affect the excitation energies by as much as 1 eV.

General information

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Organisations: Theoretical Atomic-scale Physics, Department of Physics
Contributors: Rostgaard, C., Jacobsen, K. W., Thygesen, K. S.
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Impact factor 3.813
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Impact factor 3.836
Web of Science (2016): Indexed yes
Scopus rating (2015): CiteScore 2.8 SJR 2.377 SNIP 1.13
Web of Science (2015): Impact factor 3.718
Web of Science (2015): Indexed yes
Scopus rating (2014): CiteScore 3.3 SJR 2.762 SNIP 1.316
Web of Science (2014): Impact factor 3.736
Web of Science (2014): Indexed yes
Scopus rating (2013): CiteScore 3.55 SJR 2.813 SNIP 1.326
Web of Science (2013): Impact factor 3.664
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
We use density functional theory (DFT) with a recently developed van der Waals density functional (vdW-DF) to study the adsorption of graphene on Co, Ni, Pd, Ag, Au, Cu, Pt, and Al(111) surfaces. In contrast to the local-density approximation (LDA) which predicts relatively strong binding for Ni, Co, and Pd, the vdW-DF predicts weak binding for all metals and metal-graphene distances in the range 3.40–3.72 Å. At these distances the graphene band structure as calculated with DFT and the many-body G0W0 method is basically unaffected by the substrate, in particular there is no opening of a band gap at the K point.
Modeling nanoscale gas sensors under realistic conditions: Computational screening of metal-doped carbon nanotubes

We use computational screening to systematically investigate the use of transition-metal-doped carbon nanotubes for chemical-gas sensing. For a set of relevant target molecules (CO, NH₃, and H₂S) and the main components of air (N₂, O₂, and H₂O), we calculate the binding energy and change in conductance upon adsorption on a metal atom occupying a vacancy of a (6,6) carbon nanotube. Based on these descriptors, we identify the most promising dopant candidates for detection of a given target molecule. From the fractional coverage of the metal sites in thermal equilibrium with air, we estimate the change in the nanotube resistance per doping site as a function of the target molecule concentration assuming charge transport in the diffusive regime. Our analysis points to Ni-doped nanotubes as candidates for CO sensors working under typical atmospheric conditions.
We present a computational screening study of ternary metal borohydrides for reversible hydrogen storage based on density functional theory. We investigate the stability and decomposition of alloys containing 1 alkali metal atom, Li, Na, or K (M1); and 1 alkali, alkaline earth or 3d/4d transition metal atom (M2) plus two to five (BH4)− groups, i.e., M1M2(BH4)2–5, using a number of model structures with trigonal, tetrahedral, octahedral, and free coordination of the...
metal borohydride complexes. Of the over 700 investigated structures, about 20 were predicted to form potentially stable alloys with promising decomposition energies. The M1(Al/Mn/Fe)(BH4)4, (Li/Na)Zn(BH4)3, and (Na/K)(Ni/Co)(BH4)3 alloys are found to be the most promising, followed by selected M1(Nb/Rh)(BH4)4 alloys.

**General information**

State: Published

Organisations: Theoretical Atomic-scale Physics, Department of Physics, Nano-Microstructures in Materials, Materials Research Division, Risø National Laboratory for Sustainable Energy, Electroceramics, Fuel Cells and Solid State Chemistry Division, Department of Micro- and Nanotechnology, Theoretical Nanoelectronics Group, Theory Section, Experimental Surface and Nanomaterials Physics, Center for Individual Nanoparticle Functionality, Center for Nanoteknologi, Karlsruher Institut für Technologie, Seoul National University, University of South Florida, University of Jyväskylä, University College Cork, University of California at Berkeley, French Alternative Energies and Atomic Energy Commission, University of Liverpool, University of Oslo, Swiss Federal Laboratories for Materials Science and Technology (Empa), University of New Mexico, Technical University of Denmark, University of Milan, Trinity University, Japan Advanced Institute of Science and Technology, Paul Scherrer Institute, S.N. Bose National Centre for Basic Sciences, India, Croatian Physical Society, Aarhus University, KTH - Royal Institute of Technology, University of Valladolid, University of Iceland, University of Massachusetts, University of Virginia, Iowa State University, Lomonosov Moscow State University, University of Illinois, Trinity College Dublin, Northwestern University, University of Barcelona, Delft University of Technology, University of Wisconsin-Madison, Universidad Politécnica de Madrid, University of Trieste, Johann Wolfgang Goethe-Universität Frankfurt, Universidade Federal do ABC, Nanyang Technological University, Haldor Topsoe AS, Stanford University, Gheorghe Asachi Technical University of Iasi, University of Cincinnati, Universidad del Pais Vasco, Donostia International Physics Center (DIPC), Polish Academy of Sciences, Universidade de Sao Paulo


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Web of Science (2017): Impact factor 2.843

Web of Science (2017): Indexed yes

BFI (2016): BFI-level 2

Scopus rating (2016): CiteScore 2.13 SJR 1.486 SNIP 0.964

Web of Science (2016): Impact factor 2.965

Web of Science (2016): Indexed yes

BFI (2015): BFI-level 2

Scopus rating (2015): CiteScore 1.98 SJR 1.255 SNIP 0.964

Web of Science (2015): Impact factor 2.894

Web of Science (2015): Indexed yes

BFI (2014): BFI-level 2

Scopus rating (2014): CiteScore 2.54 SJR 1.446 SNIP 1.02

Web of Science (2014): Impact factor 2.952

Web of Science (2014): Indexed yes
Inelastic scattering in metal-H-2-metal junctions
We present first-principles calculations of the dI/dV characteristics of an H-2 molecule sandwiched between Au and Pt electrodes in the presence of electron-phonon interactions. The conductance is found to decrease by a few percentages at threshold voltages corresponding to the excitation energy of longitudinal vibrations of the H-2 molecule. In the case of Pt electrodes, the transverse vibrations can mediate transport through otherwise nontransmitting Pt d channels leading to an increase in the differential conductance even though the hydrogen junction is characterized predominately by a single almost fully open transport channel. In the case of Au, the transverse modes do not affect the dI/dV because the Au d states are too far below the Fermi level. A simple explanation of the first-principles results is given using scattering theory. Finally, we compare and discuss our results in relation to experimental data.
Localized atomic basis set in the projector augmented wave method

We present an implementation of localized atomic-orbital basis sets in the projector augmented wave (PAW) formalism within the density-functional theory. The implementation in the real-space GPAW code provides a complementary basis set to the accurate but computationally more demanding grid representation. The possibility to switch seamlessly between the two representations implies that simulations employing the local basis can be fine tuned at the end of the calculation by switching to the grid, thereby combining the strength of the two representations for optimal performance. The implementation is tested by calculating atomization energies and equilibrium bulk properties of a variety of molecules and solids, comparing to the grid results. Finally, it is demonstrated how a grid-quality structure optimization can be performed with significantly reduced computational effort by switching between the grid and basis representations.
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Impact factor 3.813
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Impact factor 3.836
Web of Science (2016): Indexed yes
Scopus rating (2015): CiteScore 2.8 SJR 2.377 SNIP 1.13
Web of Science (2015): Impact factor 3.718
Web of Science (2015): Indexed yes
Scopus rating (2014): CiteScore 3.3 SJR 2.762 SNIP 1.316
Web of Science (2014): Impact factor 3.736
Web of Science (2014): Indexed yes
Scopus rating (2013): CiteScore 3.55 SJR 2.813 SNIP 1.326
Web of Science (2013): Impact factor 3.664
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): CiteScore 3.57 SJR 3.173 SNIP 1.378
Web of Science (2012): Impact factor 3.767
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): CiteScore 3.61 SJR 3.326 SNIP 1.423
Web of Science (2011): Impact factor 3.691
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 3.183 SNIP 1.447
Web of Science (2010): Impact factor 3.774
Web of Science (2010): Indexed yes
Web of Science (2009): Indexed yes
Scopus rating (2008): SJR 2.923 SNIP 1.516
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.892 SNIP 1.588
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.62 SNIP 1.468
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.126 SNIP 1.156
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.012 SNIP 1.103
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.184 SNIP 1.179
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.856 SNIP 1.841
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 3.132 SNIP 1.727
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 2.84 SNIP 1.603
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 2.789 SNIP 1.541
Original language: English
Electronic versions:
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Stability and Electronic Properties of TiO2 Nanostructures With and Without B and N Doping

We address one of the main challenges to TiO2 photocatalysis, namely band gap narrowing, by combining nanostructural changes with doping. With this aim we compare TiO2's electronic properties for small 0D clusters, 1D nanorods and nanotubes, 2D layers, and 3D surface and bulk phases using different approximations within density functional theory and GW calculations. In particular, we propose very small (R 5 Å) but surprisingly stable nanotubes with promising properties. The nanotubes are initially formed from TiO2 layers with the PTO2 structure, with the smallest (2,2) nanotube relaxing to a rutile nanorod structure. We find that quantum confinement effects, as expected, generally lead to a widening of the energy gap. However, substitutional doping with boron or nitrogen is found to give rise to (meta-)stable structures and the introduction of dopant and midgap states which effectively reduce the band gap. Boron is seen to always give rise to n-type doping while depending on the local bonding geometry, nitrogen may give rise to n-type or p-type doping. For undercoordinated TiO2 surface structures found in clusters, nanorods, nanotubes, layers and surfaces nitrogen gives rise to acceptor states while for larger clusters and bulk structures donor states are introduced.
Structure and transport properties of atomic chains and molecules

The work presented in this thesis is based on density functional theory (DFT) applied mainly to calculate conductance properties of nano-scale systems. A full characterization of Ag-oxygen chains between Ag contacts has been performed. Using spin DFT the electronic and magnetic properties of atomically thin, suspended chains containing silver and oxygen atoms in an alternating sequence has been studied. The conductances of the chains exhibit weak even-odd oscillations around an anomalously low value of 0.1G0 (G0 = 2e2/h) in agreement with experiments [1] in the long chain limit. These unusual conductance properties are explained in terms of a resonating-chain model, which takes the reflection probability and phase-shift of a single bulk-chain interface as the only input. The stability of silver-oxygen chains was studied with a thermodynamic model. This model has been developed in this work to describe tip-suspended atomically thin chains between macroscopic size electrodes. It has been tested with the use of DFT calculations on metal chains for which good agreement with experiments was obtained. To ensure the correctness of the DFT based transport calculations presented here, and in more general in the literature, a set of benchmark calculations for the Kohn-Sham elastic transmission function of representative single-molecule junctions has been performed. The transmission functions are calculated using two different density functional theory methods, namely an ultrasoft pseudopotential plane-wave code Dacapo [2] in combination with maximally localized Wannier functions and the norm-conserving pseudopotential code Siesta [3] which applies an atomic orbital basis set. For the systems studied we find that the Siesta transmission functions converge toward the plane-wave result as the Siesta basis is enlarged. Overall, we find that a double zeta polarized atomic basis is generally sufficient, and in some cases necessary, to ensure quantitative agreement with the plane-wave calculation. In a detailed DFT study of the carbon monoxide molecule between Pt electrodes, a particularly stable tilted bridge configuration is found, with a conductance of 0.5G0 over a wide range of electrode displacements. This is in agreement with the observed peak at 0.5G0 in the experimentally obtained conductance histogram for Pt/CO [4]. Also, for homogenous Pt point contacts and short chains good agreement with experiments is obtained. A study of CO in Au, Cu and Ni, reveals that the conductance for CO in the tilted bridge configuration for Ni is 0.5G0, in agreement with

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experiments [5]. For Au/CO and Cu/CO we find the effect of CO compared to the homogenous metal contacts is much smaller, in qualitative agreement with the experimental findings [5]. The observed conductance properties of Metal/CO are shown to be determined by the local d-band at the Metal apex atoms. For carbon nanotubes it is shown that the conductance may be controlled by site selective adsorption of molecules. A model to explain this behavior is verified by direct visualization of Kohn-Sham eigenchannel states. The possibility of non-carbon based nanotubes is also discussed. Both calculations of the strain energy of infinite PtO2 nanotubes that this material could be a candidate for non-carbon based nanotubes, as was recently suggested [6].

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Research output: Research › Ph.D. thesis – Annual report year: 2008

**Simulations of Mechanical Properties of CuZr and CuMg Metallic Glasses**

**General information**
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Theoretical Atomic-scale Physics, Center for Nanoteknologi
Contributors: Paduraru, A., Schiøtz, J., Jacobsen, K. W.
Publication date: Mar 2008

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Anca Paduraru.pdf
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Research output: Research › Ph.D. thesis – Annual report year: 2008

**Anomalous conductance oscillations and half-metallicity in atomic Ag-O chains**
Using spin density functional theory, we study the electronic and magnetic properties of atomically thin, suspended chains containing silver and oxygen atoms in an alternating sequence. Chains longer than 4 atoms develop a half-metallic ground state implying fully spin-polarized charge carriers. The conductances of the chains exhibit weak even-odd oscillations around an anomalously low value of 0.1G(0) (G(0) = 2e(2)/h) which coincide with the averaged experimental conductance in the long chain limit. The unusual conductance properties are explained in terms of a resonating-chain model, which takes the reflection probability and phase shift of a single bulk-chain interface as the only input. The model also explains the conductance oscillations for other metallic chains.

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Web of Science (2018): Indexed yes
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Scopus rating (2017): CiteScore 7.58 SJR 3.622 SNIP 2.464
Web of Science (2017): Impact factor 8.839
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.33 SJR 4.196 SNIP 2.61
Web of Science (2016): Impact factor 8.462
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.76 SJR 4.656 SNIP 2.538
Web of Science (2015): Impact factor 7.645
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.62 SJR 5.232 SNIP 2.71
Web of Science (2014): Impact factor 7.512
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 7.46 SJR 5.675 SNIP 2.781
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 7.19 SJR 6.292 SNIP 2.867
ISI indexed (2012): ISI indexed yes
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BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 7.02 SJR 6.314 SNIP 2.905
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 6.45 SNIP 2.757
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 6.325 SNIP 2.947
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 6.194 SNIP 2.837
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 5.95 SNIP 2.738
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 4.781 SNIP 2.443
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 4.082 SNIP 2.101
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 3.847 SNIP 2.122
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 4.661 SNIP 2.651
Web of Science (2003): Indexed yes
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 5.884 SNIP 3.375
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 5.618 SNIP 3.135
Benchmark density functional theory calculations for nanoscale conductance

We present a set of benchmark calculations for the Kohn-Sham elastic transmission function of five representative single-molecule junctions. The transmission functions are calculated using two different density functional theory methods, namely an ultrasoft pseudopotential plane-wave code in combination with maximally localized Wannier functions and the norm-conserving pseudopotential code SIESTA which applies an atomic orbital basis set. All calculations have been converged with respect to the supercell size and the number of \( k \parallel \) points in the surface plane. For all systems we find that the SIESTA transmission functions converge toward the plane-wave result as the SIESTA basis is enlarged. Overall, we find that an atomic basis with double zeta and polarization is sufficient (and in some cases, even necessary) to ensure quantitative agreement with the plane-wave calculation. We observe a systematic downshift of the SIESTA transmission functions relative to the plane-wave results. The effect diminishes as the atomic orbital basis is enlarged; however, the convergence can be rather slow.

General information

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Organisations: Theoretical Atomic-scale Physics, Department of Physics, Center for Nanoteknologi
Contributors: Strange, M., Bækgaard, I. S. B., Thygesen, K. S., Jacobsen, K. W.
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Scopus rating (2017): CiteScore 2.5 SJR 1.252 SNIP 0.926
Web of Science (2017): Impact factor 2.843
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.13 SJR 1.486 SNIP 0.964
Web of Science (2016): Impact factor 2.965
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 1.98 SJR 1.255 SNIP 0.964
Web of Science (2015): Impact factor 2.894
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.54 SJR 1.446 SNIP 1.02
Web of Science (2014): Impact factor 2.952
Comparative study of anchoring groups for molecular electronics: structure and conductance of Au-S-Au and Au-NH2-Au junctions

The electrical properties of single-molecule junctions, consisting of an organic molecule coupled to metal electrodes, are sensitive to the detailed atomic structure of the molecule-metal contact. This, in turn, is determined by the anchoring group linking the molecule to the metal. With the aim of identifying and comparing the intrinsic properties of two commonly used anchoring groups, namely thiol and amine groups, we have calculated the atomic structure and conductance traces of different Au-S-Au and Au-NH2-Au nanojunctions using density functional theory (DFT). Whereas NH2 shows a strong structural selectivity towards atop-gold configurations, S shows large variability in its bonding geometries. As a result, the conductance of the Au-NH2-Au junction is less sensitive to the structure of the gold contacts than the Au-S-Au junction. These findings support recent experiments which show that amine-bonded molecules exhibit more well-defined conductance properties than do thiol-bonded molecules.
Avalanche size scaling in sheared three-dimensional amorphous solid

We study the statistics of plastic rearrangement events in a simulated amorphous solid at T=0. Events are characterized by the energy release and the "slip volume", the product of plastic strain and system volume. Their distributions for a given system size L appear to be exponential, but a characteristic event size cannot be inferred, because the mean values of these quantities increase as L-alpha with alpha similar to 3/2. In contrast with results obtained in 2D models, we do not see simply connected avalanches. The exponent suggests a fractal shape of the avalanches, which is also evidenced by the mean fractal dimension and participation ratio.

General information
State: Published
Organisations: Experimental Surface and Nanomaterials Physics, Department of Physics, Theoretical Atomic-scale Physics, Center for Individual Nanoparticle Functionality, Center for Nanoteknologi
Contributors: Bailey, N., Schiøtz, J., Lemaître, A., Jacobsen, K. W.
Pages: 095501
Publication date: 2007
Peer-reviewed: Yes

Publication information
Journal: Physical Review Letters
Volume: 98
Atomistic simulation study of the shear-band deformation mechanism in Mg-Cu metallic glasses

We have simulated plastic deformation of a model Mg-Cu metallic glass in order to study shear banding. In uniaxial tension, we find a necking instability occurs rather than shear banding. We can force the latter to occur by deforming in plane strain, forbidding the change of length in one of the transverse directions. Furthermore, in most of the simulations a notch is used to initiate shear bands, which lie at a 45 degrees angle to the tensile loading direction. The shear bands are characterized by the Falk and Langer local measure of plastic deformation D-min(2), averaged here over volumes containing many atoms. The D-min(2) profile has a peak whose width is around 10 nm; this width is largely independent of the strain rate. Most of the simulations were, at least nominally, at 100 K, about T_g/3 for this system. The development of the shear bands takes a few tens of ps, once plastic flow has started, more or less independent of strain rate. The shear bands can also be characterized using a correlation function defined in terms of D-min(2), which, moreover, can detect incipient shear bands in cases where they do not fully form. By averaging the kinetic energy over small regions, the local temperature can be calculated, and this is seen to be higher in the shear bands by about 50-100 K. Increases in temperature appear to initiate from interactions of the shear bands with the free surfaces and with each other, and are delayed somewhat with respect to the localization of plastic flow itself. We observe a slight decrease in density, up to 1%, within the shear band, which is consistent with notions of increased free volume or disorder within a plastically deforming amorphous material.
Electronic-Structure-Based Design of Ordered Alloys

We describe some recent advances in the methodology of using electronic structure calculations for materials design. The methods have been developed for the design of ordered metallic alloys and metal alloy catalysts, but the considerations we present are relevant for the atomic-scale computational design of other materials as well. A central problem is how to treat the huge number of compounds that can be envisioned by varying the concentrations and the number of the elements involved. We discuss various strategies for approaching this problem and show how one strategy has led to the computational discovery of a promising catalytic metal alloy surface with high reactivity and low cost.

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State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
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ISSN (Print): 0883-7694
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.19 SJR 1.974 SNIP 1.559
Web of Science (2017): Impact factor 4.788
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.2 SJR 2.197 SNIP 1.613
Web of Science (2016): Impact factor 5.199
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4.68 SJR 2.6 SNIP 2.143
Web of Science (2015): Impact factor 6.06
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.61 SJR 2.048 SNIP 1.943
Web of Science (2014): Impact factor 5.667
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 3 SJR 2 SNIP 1.581
Web of Science (2013): Impact factor 5.069
Electron transport in a Pt-CO-Pt nanocontact: Density functional theory calculations

We have performed first-principles calculations for the mechanic and electric properties of pure Pt nanocontacts and a Pt contact with a single CO molecule adsorbed. For the pure Pt contacts we see a clear difference between point contacts and short chains in good agreement with experiments. We identify a tilted bridge configuration for the Pt-CO-Pt contact, which is stable and has a conductance close to $0.5G(0)$ ($G(0)=2e^2/h$), and we propose that this structure is responsible for an observed peak at $0.5G(0)$ in the conductance histogram for Pt exposed to a CO gas. We explain the main features of the transmission function for the Pt-CO-Pt contact, and show that the conductance is largely determined by the local d band at the Pt apex atoms.

General information
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Organisations: Department of Physics, Theoretical Atomic-scale Physics, Center for Nanoteknologi
Contributors: Strange, M., Thygesen, K. S., Jacobsen, K. W.
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Ratings:
Fermi level alignment in molecular nanojunctions and its relation to charge transfer

The alignment of the Fermi level of a metal electrode within the gap of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) of a molecule is a key quantity in molecular electronics, which can vary the electron transparency of a single-molecule junction by orders of magnitude. We present a quantitative analysis of the relation between this level alignment (which can be estimated from charging free molecules) and charge transfer for bipyridine and biphenyl dithiolate (BPDT) molecules attached to gold leads based on density functional theory calculations. For bipyridine the charge distribution is defined by a balance between electrostatic repulsion effects and the filling of the LUMO, where the molecule loses electrons to the leads. BPDT, on the other hand, gains electrons. As a direct consequence the Fermi level of the metal is found at the energetically higher end of the gap in the transmission function for bipyridine and at its lower end for BPDT.
An ab initio study of electron transport through nitrobenzene: The influence of leads and contacts

General information
State: Published
Organisations: Department of Physics
Contributors: Stadler, R., Thygesen, K. S., Jacobsen, K. W.
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Journal: Nanotechnology
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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.01 SJR 1.079 SNIP 0.788
Web of Science (2017): Impact factor 3.404
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.87 SJR 1.339 SNIP 0.945
Web of Science (2016): Impact factor 3.44
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.07 SJR 1.257 SNIP 1.035
Web of Science (2015): Impact factor 3.573
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.09 SJR 1.497 SNIP 1.269
Web of Science (2014): Impact factor 3.821
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.74 SJR 1.602 SNIP 1.231
Web of Science (2013): Impact factor 3.672
ISI indexed (2013): ISI Indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.34 SJR 1.861 SNIP 1.307
Web of Science (2012): Impact factor 3.842
ISI indexed (2012): ISI Indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 3.86 SJR 1.899 SNIP 1.451
Web of Science (2011): Impact factor 3.979
ISI indexed (2011): ISI Indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.844 SNIP 1.252
Web of Science (2010): Impact factor 3.652
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.809 SNIP 1.27
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.857 SNIP 1.32
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.899 SNIP 1.348
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.938 SNIP 1.364
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.958 SNIP 1.435
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.892 SNIP 1.47
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.475 SNIP 1.364
Bayesian error estimation in density-functional theory
We present a practical scheme for performing error estimates for density-functional theory calculations. The approach, which is based on ideas from Bayesian statistics, involves creating an ensemble of exchange-correlation functionals by comparing with an experimental database of binding energies for molecules and solids. Fluctuations within the ensemble can then be used to estimate errors relative to experiment on calculated quantities such as binding energies, bond lengths, and vibrational frequencies. It is demonstrated that the error bars on energy differences may vary by orders of magnitude for different systems in good agreement with existing experience.

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BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 7.58 SJR 3.622 SNIP 2.464
Web of Science (2017): Impact factor 8.839
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.33 SJR 4.196 SNIP 2.61
Web of Science (2016): Impact factor 8.462
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.76 SJR 4.656 SNIP 2.538
Web of Science (2015): Impact factor 7.645
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.62 SJR 5.232 SNIP 2.71
Web of Science (2014): Impact factor 7.512
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 7.46 SJR 5.675 SNIP 2.781
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 7.19 SJR 6.292 SNIP 2.867
Conduction Mechanism in a Molecular Hydrogen Contact

We present first principles calculations for the conductance of a hydrogen molecule bridging a pair of Pt electrodes. The transmission function has a wide plateau with $T \approx 1$ which extends across the Fermi level and indicates the existence of a single, robust conductance channel with nearly perfect transmission. Through a detailed Wannier function analysis we show that the $\text{H}_2$ bonding state is not involved in the transport and that the plateau forms due to strong hybridization between the $\text{H}_2$ antibonding state and states on the adjacent Pt atoms. The Wannier functions furthermore allow us to derive a resonant-level model for the system with all parameters determined from the fully self-consistent Kohn-Sham Hamiltonian.
Forces and conductances in a single-molecule bipyridine junction

Inspired by recent measurements of forces and conductances of bipyridine nanojunctions, we have performed density functional theory calculations of structure and electron transport in a bipyridine molecule attached between gold electrodes for seven different contact geometries. The calculations show that both the bonding force and the conductance are sensitive to the surface structure, and that both properties are in good agreement with experiment for contact geometries characterized by intermediate coordination of the metal atoms corresponding to a stepped surface. The conductance is mediated by the lowest unoccupied molecular orbital, which can be illustrated by a quantitative comparison with a one-level model. Implications for the interpretation of the experimentally determined force and conductance distributions are discussed.

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Contributors: Stadler, R., Thygesen, K. S., Jacobsen, K. W.
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Impact factor 3.813
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Impact factor 3.836
Web of Science (2016): Indexed yes
Scopus rating (2015): CiteScore 2.8 SJR 2.377 SNIP 1.13
Web of Science (2015): Impact factor 3.718
Web of Science (2015): Indexed yes
Scopus rating (2014): CiteScore 3.3 SJR 2.762 SNIP 1.316
Web of Science (2014): Impact factor 3.736
Web of Science (2014): Indexed yes
Scopus rating (2013): CiteScore 3.55 SJR 2.813 SNIP 1.326
Web of Science (2013): Impact factor 3.664
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): CiteScore 3.57 SJR 3.173 SNIP 1.378
Web of Science (2012): Impact factor 3.767
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): CiteScore 3.61 SJR 3.326 SNIP 1.423
Web of Science (2011): Impact factor 3.691
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 3.318 SNIP 1.447
Web of Science (2010): Impact factor 3.774
Web of Science (2010): Indexed yes
Web of Science (2009): Indexed yes
Scopus rating (2008): SJR 2.923 SNIP 1.516
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.892 SNIP 1.588
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.62 SNIP 1.468
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.126 SNIP 1.156
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.012 SNIP 1.103
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.184 SNIP 1.179
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.856 SNIP 1.841
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 3.132 SNIP 1.727
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 2.84 SNIP 1.603
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 2.789 SNIP 1.541

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Interference and k-point sampling in the supercell approach to phase-coherent transport - art. no. 0333401
We present a systematic study of interference and k-point sampling effects in the supercell approach to phase-coherent electron transport. We use a representative tight-binding model to show that interference between the repeated images is a small effect compared to the error introduced by using only the Gamma-point for a supercell containing (3,3) sites in the transverse plane. An insufficient k-point sampling can introduce strong but unphysical features in the transmission function which can be traced to the presence of van Hove singularities in the lead. We present a first-principles calculation of the transmission through a Pt contact which shows that the k-point sampling is also important for realistic systems.

General information
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Organisations: Theoretical Atomic-scale Physics, Department of Physics
Contributors: Thygesen, K. S., Jacobsen, K. W.
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Impact factor 3.813
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Impact factor 3.836
Web of Science (2016): Indexed yes
Scopus rating (2015): CiteScore 2.8 SJR 2.377 SNIP 1.13
Web of Science (2015): Impact factor 3.718
Web of Science (2015): Indexed yes
Scopus rating (2014): CiteScore 3.3 SJR 2.762 SNIP 1.316
Web of Science (2014): Impact factor 3.736
Web of Science (2014): Indexed yes
Scopus rating (2013): CiteScore 3.55 SJR 2.813 SNIP 1.326
Web of Science (2013): Impact factor 3.864
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): CiteScore 3.57 SJR 3.173 SNIP 1.378
Web of Science (2012): Impact factor 3.767
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): CiteScore 3.61 SJR 3.326 SNIP 1.423
Web of Science (2011): Impact factor 3.691
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 3.318 SNIP 1.447
Web of Science (2010): Impact factor 3.774
Web of Science (2010): Indexed yes
Web of Science (2009): Indexed yes
Scopus rating (2008): SJR 2.923 SNIP 1.516
Molecular transport calculations with Wannier Functions

We present a scheme for calculating coherent electron transport in atomic-scale contacts. The method combines a formally exact Green's function formalism with a mean-field description of the electronic structure based on the Kohn-Sham scheme of density functional theory. We use an accurate plane-wave electronic structure method to calculate the eigenstates which are subsequently transformed into a set of localized Wannier functions (WFs). The WFs provide a highly efficient basis set which at the same time is well suited for analysis due to the chemical information contained in the WFs. The method is applied to a hydrogen molecule in an infinite Pt wire and a benzene-dithiol (BDT) molecule between Au(111) surfaces. We show that the transmission function of BDT in a wide energy window around the Fermi level can be completely accounted for by only two molecular orbitals. (c) 2005 Elsevier B.V. All rights reserved.
Scopus rating (2017): CiteScore 1.6 SJR 0.58 SNIP 0.7
Web of Science (2017): Impact factor 1.707
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.69 SJR 0.628 SNIP 0.759
Web of Science (2016): Impact factor 1.767
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.73 SJR 0.661 SNIP 0.804
Web of Science (2015): Impact factor 1.758
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.59 SJR 0.666 SNIP 0.716
Web of Science (2014): Impact factor 1.652
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.75 SJR 0.662 SNIP 0.717
Web of Science (2013): Impact factor 2.028
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.81 SJR 0.862 SNIP 0.896
Web of Science (2012): Impact factor 1.957
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.89 SJR 0.889 SNIP 0.867
Web of Science (2011): Impact factor 1.896
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.98 SNIP 0.923
Web of Science (2010): Impact factor 2.017
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.127 SNIP 0.928
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.2 SNIP 0.885
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.092 SNIP 0.853
Scopus rating (2006): SJR 1.096 SNIP 0.973
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.287 SNIP 0.995
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.293 SNIP 0.999
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.458 SNIP 1.027
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.33 SNIP 1.022
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.411 SNIP 0.978
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.071 SNIP 0.953
Web of Science (2000): Indexed yes
Partly occupied Wannier functions
We introduce a scheme for constructing partly occupied, maximally localized Wannier functions (WFs) for both molecular and periodic systems. Compared to the traditional occupied WFs the partly occupied WFs possess improved symmetry and localization properties achieved through a bonding-antibonding closing procedure. We demonstrate the equivalence between bonding-antibonding closure and the minimization of the average spread of the WFs in the case of a benzene molecule and a linear chain of Pt atoms. The general applicability of the method is demonstrated through the calculation of WFs for a metallic system with an impurity: a Pt wire with a hydrogen molecular bridge.
Partly occupied Wannier functions: Construction and applications

We have developed a practical scheme to construct partly occupied, maximally localized Wannier functions (WFs) for a wide range of systems. We explain and demonstrate how the inclusion of selected unoccupied states in the definition of the WFs can improve both their localization and symmetry properties. A systematic selection of the relevant unoccupied states is achieved by minimizing the spread of the resulting WFs. The method is applied to a silicon cluster, a copper crystal, and a Cu(100) surface with nitrogen adsorbed. In all cases we demonstrate the existence of a set of WFs with particularly good localization and symmetry properties, and we show that this set of WFs is characterized by a maximal average localization.

General information
State: Published
Organisations: Theoretical Atomic-scale Physics, Department of Physics
Contributors: Thygesen, K. S., Hansen, L. B., Jacobsen, K. W.
Pages: 125119
Publication date: 2005
Peer-reviewed: Yes
Real-space grid implementation of the projector augmented wave method

A grid-based real-space implementation of the projector augmented wave (PAW) method of Blöchl in Phys. Rev. B 50, 17953 (1994) for density functional theory (DFT) calculations is presented. The use of uniform three-dimensional (3D) real-space grids for representing wave functions, densities, and potentials allows for flexible boundary conditions, efficient multigrid algorithms for solving Poisson and Kohn-Sham equations, and efficient parallelization using simple real-space domain-decomposition. We use the PAW method to perform all-electron calculations in the frozen core approximation, with smooth valence wave functions that can be represented on relatively coarse grids. We demonstrate the accuracy of the method by calculating the atomization energies of 20 small molecules, and the bulk modulus and lattice constants of bulk aluminum. We show that the approach in terms of computational efficiency is comparable to standard plane-wave methods, but the memory requirements are higher.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics
Pages: 035109
Publication date: 2005
Peer-reviewed: Yes

Publication information
Journal: Physical Review B Condensed Matter
Volume: 71
Issue number: 3
ISSN (Print): 0163-1829
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Impact factor 3.813
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Impact factor 3.836
Web of Science (2016): Indexed yes
Scopus rating (2015): CiteScore 2.8 SJR 2.377 SNIP 1.13
Web of Science (2015): Impact factor 3.718
Web of Science (2015): Indexed yes
Scopus rating (2014): CiteScore 3.3 SJR 2.762 SNIP 1.316
Web of Science (2014): Impact factor 3.736
Web of Science (2014): Indexed yes
Scopus rating (2013): CiteScore 3.55 SJR 2.813 SNIP 1.326
Web of Science (2013): Impact factor 3.664
ISI indexed (2013): ISI indexed yes
Stretching dependence of the vibration modes of a single-molecule Pt-H-2-Pt bridge

A conducting bridge of a single hydrogen molecule between Pt electrodes is formed in a break junction experiment. It has a conductance near the quantum unit, \( G(0) = 2e^2/h \), carried by a single channel. Using point-contact spectroscopy three vibration modes are observed and their variation upon isotope substitution is obtained. The stretching dependence for each of the modes allows uniquely classifying them as longitudinal or transversal modes. The interpretation of the experiment in terms of a Pt-H-2-Pt bridge is verified by density-functional theory calculations for the stability, vibrational modes, and conductance of the structure.
Atomistic simulations of Mg-Cu metallic glasses: Mechanical properties

The atomistic mechanisms of plastic deformation in amorphous metals are far from being understood. We have derived potential parameters for molecular dynamics simulations of Mg-Cu amorphous alloys using the Effective Medium Theory. We have simulated the formation of alloys by cooling from the melt, and have used these glassy configurations to carry out simulations of plastic deformation. These involved different compositions, temperatures (including zero), and types of deformation (uniaxial strain/pure shear), and yielded stress-strain curves and values of flow stress. Separate simulations were carried out to study specific features in the stress-strain curves associated with transitions involving internal rearrangements of atoms. Energy barriers were calculated as a function of stress, as was the plastic strain associated with events. The latter leads to a characteristic volume of an event which seems to correspond with the derivative of the barrier with respect to stress. (C) 2004 Elsevier B.V. All rights reserved.
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.76 SJR 1.694 SNIP 1.943
Web of Science (2017): Impact factor 3.414
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.669 SNIP 1.913
Web of Science (2016): Impact factor 3.094
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.01 SJR 1.742 SNIP 1.858
Web of Science (2015): Impact factor 2.647
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.32 SJR 2.235 SNIP 2.546
Web of Science (2014): Impact factor 2.567
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.86 SJR 1.868 SNIP 2.235
Web of Science (2013): Impact factor 2.409
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.5 SJR 1.744 SNIP 2.358
Web of Science (2012): Impact factor 2.108
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 2.59 SJR 1.74 SNIP 2.414
Web of Science (2011): Impact factor 2.003
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.723 SNIP 2.114
Web of Science (2010): Impact factor 2.101
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.57 SNIP 1.757
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.682 SNIP 1.859
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.326 SNIP 1.701
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.337 SNIP 1.756
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.201 SNIP 1.444
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.288 SNIP 1.625
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.42 SNIP 1.632
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.413 SNIP 1.368
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.157 SNIP 1.391
Web of Science (2001): Indexed yes
Atomic-scale insight into structure and morphology changes of MoS₂ nanoclusters in hydrotreating catalysts.

General information
State: Published
Organisations: Department of Physics, Aarhus University, Haldor Topsoe AS
Contributors: Lauritsen, J., Bollinger, M., Læsgaard, E., Jacobsen, K. W., Nørskov, J. K., Clausen, B., Topsøe, H., Besenbacher, F.
Pages: 510-522
Publication date: 2004
Peer-reviewed: Yes

Publication information
Journal: Journal of Catalysis
Volume: 221
ISSN (Print): 0021-9517
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.99 SJR 2.397 SNIP 1.85
Web of Science (2017): Impact factor 6.759
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.27 SJR 2.451 SNIP 2.142
Web of Science (2016): Impact factor 6.844
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 7.23 SJR 2.668 SNIP 2.177
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.92 SJR 2.688 SNIP 2.233
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 6.42 SJR 2.553 SNIP 2.091
Web of Science (2013): Impact factor 6.073
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 6.17 SJR 3.006 SNIP 2.257
Web of Science (2012): Impact factor 5.787
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 6.23 SJR 3.092 SNIP 2.214
Bayesian ensemble approach to error estimation of interatomic potentials

Using a Bayesian approach a general method is developed to assess error bars on predictions made by models fitted to data. The error bars are estimated from fluctuations in ensembles of models sampling the model-parameter space with a probability density set by the minimum cost. The method is applied to the development of interatomic potentials for molybdenum using various potential forms and databases based on atomic forces. The calculated error bars on elastic constants, gamma-surface energies, structural energies, and dislocation properties are shown to provide realistic estimates of the actual errors for the potentials.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Cornell University
Contributors: Frederiksen, S. L., Jacobsen, K. W., Brown, K., Sethna, J.
Pages: 165501
Publication date: 2004
Peer-reviewed: Yes

Publication information
Journal: Physical Review Letters
Volume: 93
Issue number: 16
ISSN (Print): 0031-9007
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 7.58 SJR 3.622 SNIP 2.464
Web of Science (2017): Impact factor 8.839
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.33 SJR 4.196 SNIP 2.61
Web of Science (2016): Impact factor 8.462
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.76 SJR 4.656 SNIP 2.538
Web of Science (2015): Impact factor 7.645
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.62 SJR 5.232 SNIP 2.71
Web of Science (2014): Impact factor 7.512
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 7.46 SJR 5.675 SNIP 2.781
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 7.19 SJR 6.292 SNIP 2.867
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 7.02 SJR 6.314 SNIP 2.905
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 6.45 SNIP 2.757
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 6.325 SNIP 2.947
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 6.194 SNIP 2.837
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 5.95 SNIP 2.738
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 4.781 SNIP 2.443
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 4.082 SNIP 2.101
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 3.847 SNIP 2.122
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 4.661 SNIP 2.651
Web of Science (2003): Indexed yes
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 5.884 SNIP 3.375
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 5.618 SNIP 3.135
Elastic effects behind cooperative bonding in β-sheets

We present extensive density functional theory calculations of the bonding between strands in β-sheets. We identify a significant cooperative effect whereby the interaction increases in strength with the number of strands. We show that the effect is related to a coupling between interstrand bonding and intrastrand elastic properties. It is found that a direct consequence of this coupling is that the pitch of β-sheets should contract with increasing number of strands, and we show that the effect can be observed directly in experimental data from the Protein Data Bank.

General information
State: Published
Organisations: Department of Physics
Contributors: Rossmeisl, J., Nørskov, J. K., Jacobsen, K. W.
Pages: 13140-13143
Publication date: 2004
Peer-reviewed: Yes
Matching conditions in the quasicontinuum method: Removal of the error introduced at the interface between the coarse-grained and fully atomistic region

The quasicontinuum method is a way of reducing the number of degrees of freedom in an atomistic simulation by removing the majority of the atoms in regions of slowly varying strain fields. Due to the different ways the energy of the atoms is calculated in the coarse-grained regions and the regions where all the atoms are present, unphysical forces called "ghost forces" arise at the interfaces. Corrections may be used to almost remove the ghost forces, but the correction forces are nonconservative, ruining energy conservation in dynamic simulations. We show that it is possible to formulate the quasicontinuum method without these problems by introducing a buffer layer between the two regions of space. The method is applicable to short-ranged potentials in the face-centered cubic, body-centered cubic, and hexagonal close-packed crystal structures.
Simulation of Cu-Mg metallic glass: Thermodynamics and structure

We have obtained effective medium theory interatomic potential parameters suitable for studying Cu-Mg metallic glasses. We present thermodynamic and structural results from simulations of such glasses over a range of compositions. We have produced low-temperature configurations by cooling from the melt at as slow a rate as practical, using constant temperature and pressure molecular dynamics. During the cooling process we have carried out thermodynamic analyses based on the temperature dependence of the enthalpy and its derivative, the specific heat, from which the glass transition temperature may be determined. We have also carried out structural analyses using the radial distribution function (RDF) and common neighbor analysis (CNA). Our analysis suggests that the splitting of the second peak, commonly associated with metallic glasses, in fact, has little to do with the glass transition itself, but is simply a consequence of the narrowing of peaks associated with structural features present in the liquid state. In fact, the splitting temperature for the Cu-Cu RDF is well above $T_g$. The CNA also highlights a strong similarity between the structure of the intermetallic alloys and the amorphous alloys of similar composition. We have also investigated the diffusivity in the supercooled regime. Its temperature dependence indicates fragile-liquid behavior, typical of binary metallic glasses. On the other hand, the relatively low specific-heat jump of around $1.5k_B/\text{atom}$ indicates apparent strong-liquid behavior, but this can be explained by the width of the transition due to the high cooling rates.

General information

State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Experimental Surface and Nanomaterials Physics, Department of Physics, Theoretical Atomic-scale Physics
Contributors: Bailey, N., Schiøtz, J., Jacobsen, K. W.
Number of pages: 11
Pages: 144205
Publication date: 2004
Peer-reviewed: Yes

Publication information

Journal: Physical Review B Condensed Matter
Volume: 69
Issue number: 14
ISSN (Print): 0163-1829
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Impact factor 3.813
Web of Science (2017): Indexed yes
Simulations of intergranular fracture in nanocrystalline molybdenum

Using molecular dynamics simulations we investigate the plastic deformation of nanocrystalline molybdenum with a grain size of 12 nm at high strain rates. The simulations are performed with an interatomic potential which is obtained through matching of atomic forces to a database generated with density-functional calculations. The simulations show the plastic deformation to involve both grain boundary processes and dislocation migration which in some cases lead to twin boundary formation. A large component of the strain is accommodated through the formation of cracks in the grain boundaries. This behavior is very different from what has been seen earlier in simulations of fee metals where grain boundary sliding is the dominant mechanism for very small grain sizes. (C) 2004 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
A maximum in the strength of nanocrystalline copper

We used molecular dynamics simulations with system sizes up to 100 million atoms to simulate plastic deformation of nanocrystalline copper. By varying the grain size between 5 and 50 nanometers, we show that the flow stress and thus the strength exhibit a maximum at a grain size of 10 to 15 nanometers. This maximum is because of a shift in the microscopic deformation mechanism from dislocation-mediated plasticity in the coarse-grained material to grain boundary sliding in the nanocrystalline region. The simulations allow us to observe the mechanisms behind the grain-size dependence of the strength of poly-crystalline metals.
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<td>2001</td>
<td>BFI-level 2</td>
<td>SJR 16.615, SNIP 7.018</td>
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A simple and realistic model system for studying hydrogen bonds in beta-sheets

We investigate the interaction between peptide chains at the level of state-of-the-art ab initio density functional theory. We propose an interacting periodic polypeptide model for studying the interactions in beta-sheets and apply this to glycine and alanine peptide chains in both parallel and antiparallel structures. The calculated structures of alanine are compared to x-ray structures of beta-sheets and the model is found to reproduce the geometry of the hydrogen bonds very well both concerning parallel and antiparallel beta-sheets. We investigate the structures of both the N-H...O=C and the C-alpha-H...O=C hydrogen bonds. The former is thoroughly investigated, whereas the structure of the latter still is the subject of much discussion. We show that the hydrogen bonds between peptide chains are considerably weaker than what is found in studies of smaller models, e.g., the N-methylacetamide molecule. By molecular mechanics calculations we study the effect of twisting, which is not included in our model. We estimate its contribution to the interaction energy to be small.

General information
State: Published
Organisations: Theoretical Atomic-scale Physics, Department of Physics, Novo Nordisk A/S, H. Lundbeck A/S
Pages: 9783-9794
Publication date: 2003
Peer-reviewed: Yes

Publication information
Journal: Journal of Chemical Physics
Volume: 118
Issue number: 21
ISSN (Print): 0021-9606
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 2.5 SJR 1.252 SNIP 0.926
Web of Science (2017): Impact factor 2.843
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.13 SJR 1.486 SNIP 0.964
Web of Science (2016): Impact factor 2.965
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 1.98 SJR 1.255 SNIP 0.964
Web of Science (2015): Impact factor 2.894
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.54 SJR 1.446 SNIP 1.02
Web of Science (2014): Impact factor 2.952
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.95 SJR 1.559 SNIP 1.174
Web of Science (2013): Impact factor 3.122
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.86 SJR 1.832 SNIP 1.137
Web of Science (2012): Impact factor 3.164
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Atomic and electronic structure of MoS2 nanoparticles

Using density-functional theory (DFT) we present a detailed theoretical study of MoS2 nanoparticles. We focus on the edge structures, and a number of different edge terminations are investigated. Several, but not all, of these configurations have one-dimensional metallic states localized at the edges. The electronic structure of the edge states is studied and we discuss their influence on the chemical properties of the edges. In particular, we study the reactivity towards hydrogen and show that hydrogen may form stable chemical bonds with both the two low-Miller indexed edges of MoS2. A model for calculating Gibbs free energy of the edges in terms of the DFT energies is also presented. This model allows us to determine the stable edge structure in thermodynamic equilibrium under different conditions. We find that both the
insulating and metallic edges may be stable depending on the temperature and the composition of the gas phase. Using the Tersoff-Hamann formalism, scanning-tunneling microscopy (STM) images of the edges are simulated for direct comparison with recent STM experiments. In this way we identify the experimentally observed edge structure.

**General information**
- **State:** Published
- **Organisations:** Department of Physics, Theoretical Atomic-scale Physics
- **Contributors:** Bollinger, M., Jacobsen, K. W., Nørskov, J. K.
- **Pages:** 085410
- **Publication date:** 2003
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  - BFI (2018): BFI-level 1
  - Web of Science (2018): Indexed yes
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  - Web of Science (2017): Impact factor 3.813
  - Web of Science (2017): Indexed yes
  - Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
  - Web of Science (2016): Impact factor 3.836
  - Web of Science (2016): Indexed yes
  - Scopus rating (2015): CiteScore 2.8 SJR 2.377 SNIP 1.13
  - Web of Science (2015): Indexed yes
  - Scopus rating (2014): CiteScore 3.3 SJR 2.762 SNIP 1.316
  - Web of Science (2014): Impact factor 3.736
  - Web of Science (2014): Indexed yes
  - Scopus rating (2013): CiteScore 3.55 SJR 2.813 SNIP 1.326
  - Web of Science (2013): Impact factor 3.664
  - ISI indexed (2013): ISI indexed yes
  - Web of Science (2013): Indexed yes
  - Scopus rating (2012): CiteScore 3.57 SJR 3.173 SNIP 1.378
  - Web of Science (2012): Impact factor 3.767
  - ISI indexed (2012): ISI indexed yes
  - Web of Science (2012): Indexed yes
  - Scopus rating (2011): CiteScore 3.61 SJR 3.326 SNIP 1.423
  - Web of Science (2011): Impact factor 3.691
  - ISI indexed (2011): ISI indexed yes
  - Web of Science (2011): Indexed yes
  - Scopus rating (2010): SJR 3.318 SNIP 1.447
  - Web of Science (2010): Impact factor 3.774
  - Web of Science (2010): Indexed yes
  - Web of Science (2009): Indexed yes
  - Scopus rating (2008): SJR 2.923 SNIP 1.516
  - Web of Science (2008): Indexed yes
  - Scopus rating (2007): SJR 2.892 SNIP 1.588
  - Web of Science (2007): Indexed yes
  - Scopus rating (2006): SJR 2.62 SNIP 1.468
  - Web of Science (2006): Indexed yes
  - Scopus rating (2005): SJR 2.126 SNIP 1.156
  - Web of Science (2005): Indexed yes
The natural amino acids have different preferences of occurring in specific types of secondary protein structure. Simulations are performed on periodic model β-sheets of 14 different amino acids, at the level of density functional theory, employing the generalized gradient approximation. We find that the statistically observed β-sheet propensities correlate very well with the calculated binding energies. Analysis of the calculations shows that the β-sheet propensities are determined by the local flexibility of the individual polypeptide strands.
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 12.81 SJR 6.775 SNIP 2.63
Web of Science (2015): Impact factor 13.038
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 11.92 SJR 6.294 SNIP 2.587
Web of Science (2014): Impact factor 12.113
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 11.38 SJR 5.993 SNIP 2.466
Web of Science (2013): Impact factor 11.444
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 10.37 SJR 6.211 SNIP 2.38
Web of Science (2012): Impact factor 10.677
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 9.94 SJR 5.478 SNIP 2.321
Web of Science (2011): Impact factor 9.907
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 5.167 SNIP 2.138
Web of Science (2010): Impact factor 9.023
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 5.06 SNIP 2.16
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 4.662 SNIP 2.252
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 4.413 SNIP 2.223
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 3.841 SNIP 2.203
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 3.421 SNIP 2.236
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 3.223 SNIP 2.345
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 3.506 SNIP 2.15
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 3.972 SNIP 2.163
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 3.438 SNIP 2.133

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10.1021/ja0359658
Chemistry of one-dimensional metallic edge states in MoS$_2$ nanoclusters

General information
State: Published
Organisations: Department of Physics, Aarhus University, Technical University of Denmark, Haldor Topsoe AS
Contributors: Lauritsen, J., Nyberg, M., Vang, R., Bollinger, M., Clausen, B., Topsøe, H., Jacobsen, K. W., Nørskov, J. K., Besenbacher, F.
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.01 SJR 1.079 SNIP 0.788
Web of Science (2017): Impact factor 3.404
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.87 SJR 1.339 SNIP 0.945
Web of Science (2016): Impact factor 3.44
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.07 SJR 1.257 SNIP 1.035
Web of Science (2015): Impact factor 3.573
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.09 SJR 1.497 SNIP 1.269
Web of Science (2014): Impact factor 3.821
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.74 SJR 1.602 SNIP 1.231
Web of Science (2013): Impact factor 3.672
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.34 SJR 1.861 SNIP 1.307
Web of Science (2012): Impact factor 3.842
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 3.86 SJR 1.899 SNIP 1.451
Web of Science (2011): Impact factor 3.979
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.844 SNIP 1.252
Web of Science (2010): Impact factor 3.652
Conductance calculations with a wavelet basis set

We present a method based on density functional theory (DFT) for calculating the conductance of a phase-coherent system. The metallic contacts and the central region where the electron scattering occurs, are treated on the same footing taking their full atomic and electronic structure into account. The linear-response conductance is calculated from the Green’s function which is represented in terms of a system-independent basis set containing wavelets with compact support. This allows us to rigorously separate the central region from the contacts and to test for convergence in a systematic way. The method supports the use of both norm-conserving and ultrasoft pseudopotentials. We use the method to study the effect of adsorbates on the conductance of an infinitely long, atomically thin Al wire, and find that hydrogen and oxygen effectively reduce the conductance of the wire by one and two conductance quanta, respectively.

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Organisations: Theoretical Atomic-scale Physics, Department of Physics
Contributors: Thygesen, K. S., Bollinger, M., Jacobsen, K. W.
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Web of Science (2017): Impact factor 3.813
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Impact factor 3.836
Web of Science (2016): Indexed yes
Scopus rating (2015): CiteScore 2.8 SJR 2.377 SNIP 1.13
Web of Science (2015): Impact factor 3.718
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Scopus rating (2014): CiteScore 3.3 SJR 2.762 SNIP 1.316
Web of Science (2014): Impact factor 3.736
Web of Science (2014): Indexed yes
Scopus rating (2013): CiteScore 3.55 SJR 2.813 SNIP 1.326
Web of Science (2013): Impact factor 3.664
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): CiteScore 3.57 SJR 3.173 SNIP 1.378
Web of Science (2012): Impact factor 3.767
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): CiteScore 3.61 SJR 3.326 SNIP 1.423
Web of Science (2011): Impact factor 3.691
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 3.318 SNIP 1.447
Web of Science (2010): Impact factor 3.774
Web of Science (2010): Indexed yes
Web of Science (2009): Indexed yes
Scopus rating (2008): SJR 2.923 SNIP 1.516
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.892 SNIP 1.588
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.62 SNIP 1.468
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.126 SNIP 1.156
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.012 SNIP 1.103
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.184 SNIP 1.179
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.856 SNIP 1.841
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 3.132 SNIP 1.727
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 2.84 SNIP 1.603
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 2.789 SNIP 1.541

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Electronic versions: Thygesen.pdf

DOIs: 10.1103/PhysRevB.67.115404

URLs:
Density functional theory studies of screw dislocation core structures in bcc metals

The core structures of (1 1 1) screw dislocations in bcc metals are studied using density functional theory in the local-density approximation. For Mo and Fe, direct calculations of the core structures show the cores to be symmetric with respect to 180 degrees rotations around an axis perpendicular to the dislocation line. The magnetic moment in the Fe core is shown to be reduced relative to the bulk value. Calculations of gamma surfaces and the elastic constants B, C' and c(44) are reported for Fe and all group VB and VIB metals. Using a criterion suggested by Vitek and Duesbery the calculations point to symmetric core structures for all the studied metals.
Four-atom period in the conductance of monatomic Al wires

We present first-principles calculations based on density functional theory for the conductance of monatomic Al wires between Al(111) electrodes. In contrast to the even-odd oscillations observed in other metallic wires, the conductance of the Al wires is found to oscillate with a period of four atoms as the length of the wire is varied. Although local charge neutrality can account for the observed period, it leads to an incorrect phase. We explain the conductance behavior using a resonant transport model based on the electronic structure of the infinite wire.
Pareto-optimal alloys

Large databases that can be used in the search for new materials with specific properties remain an elusive goal in materials science. The problem is complicated by the fact that the optimal material for a given application is usually a compromise between a number of materials properties and the cost. In this letter we present a database consisting of the lattice parameters, bulk moduli, and heats of formation for over 64 000 ordered metallic alloys, which has been established by direct first-principles density-functional-theory calculations. Furthermore, we use a concept from economic theory, the Pareto-optimal set, to determine optimal alloy solutions for the compromise between low compressibility, high stability, and cost.
Adsorption-induced restructuring of gold nanochains

The chemical properties of single-atomic chains of gold atoms are investigated using density functional calculations. The nanochains are shown to be unusually chemically active with strong chemisorption of oxygen atoms and carbon monoxide. The chemisorption energies vary significantly with the strain/stress conditions for the chain. Oxygen atoms are found to energetically prefer to get incorporated into a chain forming a new type of gold-oxygen nanochain with a conductance of one quantum unit. We suggest that the long bond lengths observed in electron microscopy investigations of gold chains can be due to oxygen incorporation.
An object-oriented scripting interface to a legacy electronic structure code

The authors have created an object-oriented scripting interface to a mature density functional theory code. The interface gives users a high-level, flexible handle on the code without rewriting the underlying number-crunching code. The authors also discuss design issues and the advantages of homogeneous interfaces.
Atomic-scale structure of dislocations revealed by scanning tunneling microscopy and molecular dynamics

The intersection between dislocations and a Ag(111) surface has been studied using an interplay of scanning tunneling microscopy (STM) and molecular dynamics. Whereas the STM provides atomically resolved information about the surface structure and Burgers vectors of the dislocations, the simulations can be used to determine dislocation structure and orientation in the near-surface region. In a similar way, the subsurface structure of other extended defects can be studied. The simulations show dislocations to reorient the partials in the surface region leading to an increased splitting width at the surface, in agreement with the STM observations. Implications for surface-induced cross slip are discussed.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Theoretical Atomic-scale Physics, Aarhus University, Free University of Berlin
Contributors: Christiansen, J., Morgenstern, K., Schiøtz, J., Jacobsen, K. W., Braun, K., Rieder, K., Laegsgaard, E., Besenbacher, F.
Number of pages: 4
Pages: 206106
Combined electronic structure and evolutionary search approach to materials design

We show that density functional theory calculations have reached an accuracy and speed making it possible to use them in conjunction with an evolutionary algorithm to search for materials with specific properties. The approach is illustrated by finding the most stable four component alloys out of the 192 016 possible fcc and bcc alloys that can be constructed out of 32 different metals. A number of well known and new "super alloys" are identified in this way.

General information

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Organisations: Department of Physics, Theoretical Atomic-scale Physics
Contributors: Johannesson, G. H., Bligaard, T., Ruban, A., Skriver, H. L., Jacobsen, K. W., Nørskov, J. K.
Pages: 255506
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BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 7.58 SJR 3.622 SNIP 2.464
Web of Science (2017): Impact factor 8.839
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.33 SJR 4.196 SNIP 2.61
Web of Science (2016): Impact factor 8.462
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.76 SJR 4.656 SNIP 2.538
Web of Science (2015): Impact factor 7.645
Web of Science (2015): Indexed yes
Computational materials science: Nanoscale plasticity
How does plastic deformation of polycrystalline materials with grain sizes less than 100 nm look at the atomic scale? A large-scale molecular dynamics simulation of nanocrystalline aluminium reveals some surprising behaviour.

General information
State: Published
Organisations: Department of Physics
Contributors: Jacobsen, K. W., Schiøtz, J.
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Peer-reviewed: Yes

Publication information
Journal: Nature Materials
Volume: 1
Issue number: 1
ISSN (Print): 1476-1122
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BFI (2018): BFI-level 3
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 25.47 SJR 18.263 SNIP 8.977
Web of Science (2017): Impact factor 39.235
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 23.67 SJR 18.013 SNIP 9.04
Web of Science (2016): Impact factor 39.737
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Web of Science (2015): Impact factor 38.891
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 23.23 SJR 14.956 SNIP 8.905
Web of Science (2014): Impact factor 36.503
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 23.3 SJR 16.726 SNIP 9.171
Web of Science (2013): Impact factor 36.425
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 21.29 SJR 18.482 SNIP 8.331
Web of Science (2012): Impact factor 35.749
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 19.84 SJR 17.79 SNIP 7.876
Web of Science (2011): Impact factor 32.841
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 18.404 SNIP 7.654
Web of Science (2010): Impact factor 29.92
Object oriented scripting interface to a legacy electronic structure code

General information
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Organisations: Department of Physics
Contributors: Bahn, S. R., Jacobsen, K. W.
Pages: 56
Publication date: 2002
Peer-reviewed: Yes

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Journal: Computing in Science & Engineering
Volume: 4
ISSN (Print): 1521-9615
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2 SJR 0.748 SNIP 1.374
Web of Science (2017): Impact factor 1.074
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.69 SJR 0.503 SNIP 1.373
Web of Science (2016): Impact factor 2.074
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.56 SJR 0.599 SNIP 1.418
Web of Science (2015): Impact factor 1.361
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.42 SJR 0.478 SNIP 1.244
Web of Science (2014): Impact factor 0.99
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.55 SJR 0.497 SNIP 1.549
Web of Science (2013): Impact factor 1.248
The quasicontinuum method revisited;: in "Challenges in Molecular Simulations", ed. D. Mac Kernan

General information
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Organisations: Department of Physics
Contributors: Mortensen, J. J., Schiøtz, J., Jacobsen, K. W.
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Peer-reviewed: Unknown

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Journal: SIMU Newsletter
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Original language: English
Source: orbit
Source-ID: 132425
Research output: Research - peer-review › Journal article – Annual report year: 2002

Adsorption-induced step formation
Through an interplay between density functional calculations, Monte Carlo simulations and scanning tunneling microscopy experiments, we show that an intermediate coverage of CO on the Pt(110) surface gives rise to a new rough equilibrium structure with more than 50% step atoms. CO is shown to bind so strongly to low-coordinated Pt atoms that it can break Pt-Pt bonds and spontaneously form steps on the surface. It is argued that adsorption-induced step formation may be a general effect, in particular at high gas pressures and temperatures.

General information
State: Published
Calculation of quantum tunneling for a spatially extended defect: The dislocation kink in copper has a low effective mass

Several experiments indicate that there are atomic tunneling defects in plastically deformed metals. How this is possible has not been clear, given the large mass of the metal atoms. Using a classical molecular-dynamics calculation, we determine the structures, energy barriers, effective masses, and quantum tunneling rates for dislocation kinks and jogs in copper screw dislocations. We find that jogs are unlikely to tunnel, but the kinks should have large quantum fluctuations. The kink motion involves hundreds of atoms each shifting a tiny amount, leading to a small effective mass and tunneling barrier.
Original language: English
Keywords: SYSTEMS, INSTANTON APPROACH, SOLIDS, STRESS, POLYACETYLENE, CRYSTALS, SLOW 2-LEVEL FLUCTUATORS, METALLIC GLASSES, POINT-CONTACT, TEMPERATURE
Chain formation of metal atoms

The possibility of formation of single-atomic chains by manipulation of nanocontacts is studied for a selection of metals (Ni, Pd, Pt, Cu, Ag, Au). Molecular dynamics simulations show that the tendency for chain formation is strongest for Au and Pt. Density functional theory calculations indicate that the metals which form chains exhibit pronounced many-atom interactions with strong bonding in low coordinated systems.
A scanning tunneling microscope supplemented with a force sensor is used to study the mechanical properties of a novel metallic nanostructure: a freely suspended chain of single gold atoms. We find that the bond strength of the nanowire is about twice that of a bulk metallic bond. We perform ab initio calculations of the force at chain fracture and compare quantitatively with experimental measurements. The observed mechanical failure and nanoelastic processes involved during atomic wire fabrication are investigated using molecular dynamics simulations, and we find that the total effective stiffness of the nanostructure is strongly affected by the detailed local atomic arrangement at the chain bases.
One-dimensional metallic edge states in MoS2
By the use of density functional calculations it is shown that the edges of a two-dimensional slab of insulating MoS2 exhibit several metallic states. These edge states can be viewed as one-dimensional conducting wires, and we show that they can be observed directly using scanning tunneling microscopy for single-layer MoS2 nanoparticles grown on a support.

General information
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Organisations: Department of Physics, Theoretical Atomic-scale Physics, Aarhus University
Contributors: Bollinger, M., Lauritsen, J., Jacobsen, K. W., Nørskov, J. K., Helveg, S., Besenbacher, F.
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BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 7.58 SJR 3.622 SNIP 2.464
Web of Science (2017): Impact factor 8.839
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.33 SJR 4.196 SNIP 2.61
Web of Science (2016): Impact factor 8.462
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.76 SJR 4.656 SNIP 2.538
Web of Science (2015): Impact factor 7.645
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.62 SJR 5.232 SNIP 2.71
Web of Science (2014): Impact factor 7.512
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 7.46 SJR 5.675 SNIP 2.781
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 7.19 SJR 6.292 SNIP 2.867
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 7.02 SJR 6.314 SNIP 2.905
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 6.45 SNIP 2.757
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 6.325 SNIP 2.947
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 6.194 SNIP 2.837
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 5.95 SNIP 2.738
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 4.781 SNIP 2.443
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 4.082 SNIP 2.101
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 3.847 SNIP 2.122
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 4.661 SNIP 2.651
Web of Science (2003): Indexed yes
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 5.884 SNIP 3.375
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 5.618 SNIP 3.135
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 5.771 SNIP 2.941
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Research output: Research - peer-review; Journal article – Annual report year: 2001
Comment on "density functional simulation of a breaking nanowire" Nakamura et al. reply

General information
State: Published
Organisations: Theoretical Nanoelectronics Group, Theory Section, Department of Micro- and Nanotechnology, Department of Physics, Theoretical Atomic-scale Physics, Anan College of Technology
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Journal: Physical Review Letters
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Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 7.58 SJR 3.622 SNIP 2.464
Web of Science (2017): Impact factor 8.839
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.33 SJR 4.196 SNIP 2.61
Web of Science (2016): Impact factor 8.462
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.76 SJR 4.656 SNIP 2.538
Web of Science (2015): Impact factor 7.645
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.62 SJR 5.232 SNIP 2.71
Web of Science (2014): Impact factor 7.512
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 7.46 SJR 5.675 SNIP 2.781
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 7.19 SJR 6.292 SNIP 2.867
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 7.02 SJR 6.314 SNIP 2.905
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 6.45 SNIP 2.757
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 6.325 SNIP 2.947
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 6.194 SNIP 2.837
Web of Science (2008): Indexed yes
Determination of the rate of cross slip of screw dislocations

The rate for cross slip of screw dislocations during annihilation of screw dipoles in copper is determined by molecular dynamics simulations. The temperature dependence of the rate is seen to obey an Arrhenius behavior in the investigated temperature range: 225-375 K. The activation energy and the effective attempt frequency can therefore be extracted from the simulations. The transition state energy for the annihilation process is calculated by identifying the transition state using the nudged elastic band path technique. The two activation energies agree very well, indicating that transition state theory is applicable for this type of process.

General information
State: Published
Organisations: Department of Physics, Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy, Theoretical Atomic-scale Physics
Contributors: Vegge, T., Rasmussen, T., Leffers, T., Pedersen, O. B., Jacobsen, K. W.
Pages: 3866-3869
Publication date: 2000
Peer-reviewed: Yes

Publication information
Journal: Physical Review Letters
Volume: 85
Issue number: 18
ISSN (Print): 0031-9007
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 7.58 SJR 3.622 SNIP 2.464
Web of Science (2017): Impact factor 8.839
Simulation of structure and annihilation of screw dislocation dipoles
Large scale atomistic simulations are used to investigate the properties of screw dislocation dipoles in copper. Spontaneous annihilation is observed for dipole heights less than 1 nm. Equilibrated dipoles of heights larger than 1 nm adopt a skew configuration due to the elastic anisotropy of Cu. The equilibrium splitting width of the screw dislocations decreases with decreasing dipole height, as expected from elasticity theory. The energy barriers, and corresponding transition states for annihilation of stable dipoles are determined for straight and for flexible dislocations for dipole heights up to 5.2 nm. In both cases the annihilation is initiated by cross-slip of one of the dislocations. For straight dislocations the activation energy shows a linear dependence on the inverse dipole height, and for flexible dislocations the dependence is roughly linear for the dipoles investigated.

Surface chemistry in three dimensions: CO dissociation between two surfaces
Based on self-consistent density functional calculations it is shown that a new dissociation process for CO adsorbed on a Ru(0001) surface is made possible when the distance to a second Ru(0001) surface placed just above it is below some critical value. This '3D' process is more facile than the usual single surface ('2D') process because indirect adsorbate-adsorbate interactions in the transition state are absent in the '3D' case. The prospects for STM-induced single molecule chemistry and for '3D' catalysts are discussed. (C) 2000 Elsevier Science B.V. All rights reserved.
Atomic-scale modeling of the deformation of nanocrystalline metals

General information
State: Published
Organisations: Department of Physics
Contributors: Schiøtz, J., Vegge, T., Jacobsen, K. W.
Pages: 299-308
Publication date: 1999

Host publication information
Title of host publication: Multiscale Modelling of Materials
Place of publication: Warrendale, PA, USA
Publisher: Materials Research Society
ISBN (Print): 1-55899-444-0
(Materials Research Society symposium proceedings, 538).
Source: orbit
Source-ID: 173639
Research output: Research - peer-review » Article in proceedings – Annual report year: 1999

Atomic-scale simulations of the mechanical deformation of nanocrystalline metals

Nanocrystalline metals, i.e., metals in which the grain size is in the nanometer range, have a range of technologically interesting properties including increased hardness and yield strength. We present atomic-scale simulations of the plastic behavior of nanocrystalline copper. The simulations show that the main deformation mode is sliding in the grain boundaries through a large number of uncorrelated events, where a few atoms (or a few tens of atoms) slide with respect to each other. Little dislocation activity is seen in the grain interiors. The localization of the deformation to the grain boundaries leads to a hardening as the grain size is increased (reverse Hall-Fetch effect), implying a maximum in hardness for a grain size above the ones studied here. We investigate the effects of varying temperature, strain rate, and porosity, and discuss the relation to recent experiments. At increasing temperatures the material becomes softer in both the plastic and elastic regime. Porosity in the samples result in a softening of the material; this may be a significant effect in many experiments. [S0163-1829(99)05941-X].

General information
State: Published
Organisations: Experimental Surface and Nanomaterials Physics, Department of Physics, Theoretical Atomic-scale Physics
Contributors: Schiøtz, J., Vegge, T., Di Tolla, F., Jacobsen, K. W.
Pages: 11971-11983
Publication date: 1999
Density Functional Simulation of a Breaking Nanowire

We study the deformation and breaking of an atomic-sized sodium wire using density functional simulations. The wire deforms through sudden atomic rearrangements and smoother atomic displacements. The conductance of the wire exhibits plateaus at integer values in units of $2e^2/h$ corresponding to a specific number of eigenchannels. The transitions between plateaus can be abrupt in connection with structural rearrangements or extend over a few $\alpha$ of elongation. The interplay between conductance modes and structural deformation is discussed by means of the eigenchannel transmission probabilities.
Enhancement of surface self-diffusion of platinum atoms by adsorbed hydrogen

General information
State: Published
Organisations: Department of Physics, Aarhus University
Pages: 134
Publication date: 1999
Peer-reviewed: Yes

Publication information
Journal: Nature
Volume: 398
ISSN (Print): 0028-0836
Ratings:
BFI (2018): BFI-level 3
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 14.59
Web of Science (2017): Impact factor 19.181
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 13.33
Web of Science (2016): Impact factor 19.304
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 14.38
Web of Science (2015): Impact factor 17.184
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 14.22
Web of Science (2014): Impact factor 14.547
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 14.96
Web of Science (2013): Impact factor 15.295
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 14.01
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
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Scopus rating (2011): CiteScore 13.96
Web of Science (2011): Impact factor
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Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Mechanisms of self-diffusion on Pt(110)
The self-diffusion of Pt on the missing row reconstructed Pt(110) surface is discussed based on density functional calculations of activation energy barriers. Different competing diffusion mechanisms are considered and we show that several different diffusion paths along the reconstruction troughs are of relevance. The analysis leads to another interpretation of the recently observed double jumps at the Pt(110) surface. [S0163-1829(99)51732-3].

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics
Contributors: Lorensen, H. Q., Nørskov, J. K., Jacobsen, K. W.
Pages: R5149-R5152
Publication date: 1999
Peer-reviewed: Yes

Publication information
Journal: Physical Review B
Volume: 60
Issue number: 8
ISSN (Print): 2469-9950
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Impact factor 3.813
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Impact factor 3.836
Web of Science (2016): Indexed yes
Scopus rating (2015): CiteScore 2.8 SJR 2.377 SNIP 1.13
Web of Science (2015): Impact factor 3.718
Web of Science (2015): Indexed yes
Scopus rating (2014): CiteScore 3.3 SJR 2.762 SNIP 1.316
Web of Science (2014): Impact factor 3.736
Web of Science (2014): Indexed yes
Scopus rating (2013): CiteScore 3.55 SJR 2.813 SNIP 1.326
Web of Science (2013): Impact factor 3.664
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): CiteScore 3.57 SJR 3.173 SNIP 1.378
Web of Science (2012): Impact factor 3.767
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): CiteScore 3.61 SJR 3.326 SNIP 1.423
Web of Science (2011): Impact factor 3.691
Oxygen adsorption on Pt(110)-(1x2): new high-coverage structures
From an interplay between scanning tunneling microscopy (STM) experiments and density functional theory (DFT) calculations, a comprehensive picture is obtained for oxygen adsorption on the Pt(110)-(1 x 2) surface, from single isolated oxygen atoms chemisorbed in FCC sites along the platinum ridges to the formation of a new high-coverage oxide-like structure with a local coverage of two oxygen atoms per platinum surface atom. We find that the repulsive O-O interactions for the O/Pt(110) system are compensated by an effective O-O attractive interaction originating from a strong coupling between oxygen adsorption and platinum lattice distortions. (C) 1999 Elsevier Science B.V. All rights reserved.

General information
State: Published
Organisations: Department of Physics, Aarhus University
Pages: L533-L539
Publication date: 1999
Peer-reviewed: Yes
A theoretical study of adsorption and dissociation on metal surfaces

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics
Contributors: Mortensen, J. J., Jacobsen, K. W., Nørskov, J. K.
Publication date: Apr 1998

Publication information
Place of publication: Kgs. Lyngby, Denmark
Publisher: Technical University of Denmark (DTU)
Original language: English
Source: orbit
Source-ID: 276599

Effects of anisotropic diffusion and finite island sizes in homoepitaxial growth Pt on Pt(100)-hex

The diffusion, nucleation, and growth of Pt on the hexagonally reconstructed Pt(100)-hex surface are investigated. By means of Scanning Tunneling Microscopy (STM), the positions, sizes, and number densities of monoatomically high, rectangular, reconstructed Pt islands, formed in the submonolayer coverage regime, have been determined for substrate temperatures in the range T = 318-497 K and adatom deposition rates from R=4 x 10(-5) to 7 x 10(-3) site(-1) s(-1). The measurements are compared to the results of kinetic Monte Carlo (KMC) simulations and rate equation theory.

The Pt(100)-hex surface exhibits a height modulation caused by the misfit between the topmost quasi-hexagonal layer and the quadratic substrate, resulting in a highly anisotropic large scale surface morphology with six-atom wide channels running along the [1(1) over bar0] direction. From an autocorrelation analysis of the determined island positions, it is revealed that the islands are distributed with long/short correlation lengths along, perpendicular to the reconstruction channels. The autocorrelation analysis allows us to quantify the degree of anisotropy in adatom diffusion. Island size distributions obtained at different temperatures are found to collapse onto a single scaling curve also in the present case of strongly anisotropic diffusion. By comparison to similar curves derived from KMC simulations in a model incorporating anisotropic diffusion and finite island sizes, it is concluded that the critical island size is i=1 and that the mobility of dimers is negligible. Furthermore, an early onset of island coalescence is revealed. From the scaling of the measured saturation island density, N-x similar to(R/h)(chi), where h = v exp(-E-d/k(B)T) is the adatom hopping rate, an effective barrier for diffusion of E-d=0.43 eV and a scaling exponent of chi=0.27 are obtained. From KMC simulations the scaling of N-x is found to be influenced by the finite extent of the islands when diffusion is anisotropic. This is due to the increased ability of the islands to capture adatoms as they grow to cover more diffusion channels. Rate equations incorporating this effect are solved, and a scaling exponent of chi=1/3 is derived in contrast to the chi=1/4 obtained for a 1-D point-island model. (C) 1998 Elsevier Science B.V.

General information
State: Published
Organisations: Department of Physics, Aarhus University
Contributors: Mortensen, J. J., Linderoth, T., Jacobsen, K. W., Lægsgaard, E., Stensgaard, I., Besenbacher, F.
Pages: 290-313
Mechanical deformation of atomic-scale metallic contacts: Structure and mechanisms

We have simulated the mechanical deformation of atomic-scale metallic contacts under tensile strain using molecular dynamics and effective medium theory potentials. The evolution of the structure of the contacts and the underlying deformation mechanisms are described along with the calculated electronic conductance. Various defects such as intersecting stacking faults, local disorder, and vacancies are created during the deformation. Disordered regions act as weak spots that reduce the strength of the contacts. The disorder tends to anneal out again during the subsequent atomic rearrangements, but vacancies can be permanently present. The transition states and energies for slip mechanisms have been determined using the nudged elastic band method, and we find a size-dependent crossover from a dislocation-mediated slip to a homogeneous slip when the contact diameter becomes less than a few nm. We show that the results measured in a nanocontact experiment depend significantly on the elastic stiffness of the experimental apparatus. For a soft setup, some of the atomic rearrangements might not be detected, whereas others are amplified.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics
Contributors: Sørensen, M. R., Brandbyge, M., Jacobsen, K. W.
Pages: 3283-3294
Publication date: 1998
Peer-reviewed: Yes

Publication information
Journal: Physical Review B
Volume: 57
Issue number: 6
ISSN (Print): 2469-9950
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Impact factor 3.813
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Impact factor 3.836
Web of Science (2016): Indexed yes
Scopus rating (2015): CiteScore 2.8 SJR 2.377 SNIP 1.13
Web of Science (2015): Impact factor 3.718
Web of Science (2015): Indexed yes
Scopus rating (2014): CiteScore 3.3 SJR 2.762 SNIP 1.316
Simulations of mechanics and structure of nanomaterials - from nanoscale to coarser scales

General information
State: Published
Organisations: Department of Physics
Contributors: Schiøtz, J., Vegge, T., Di Tolla, F., Jacobsen, K. W.
Number of pages: 133
Publication date: 1998

Host publication information
Title of host publication: Modelling of Structure and Mechanics of Materials from Microscale to Product
Source: orbit
Source-ID: 171387
Research output: Research - peer-review › Article in proceedings – Annual report year: 1998

Softening of nanocrystalline metals at very small grain sizes

General information
State: Published
Organisations: Department of Physics
Contributors: Schiøtz, J., Di Tolla, F., Jacobsen, K. W.
Pages: 561
Publication date: 1998
Peer-reviewed: Yes

Publication information
Journal: Nature
Volume: 391
ISSN (Print): 0028-0836
Ratings:
BFI (2018): BFI-level 3
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 14.59
Web of Science (2017): Impact factor 19.181
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 13.33
Web of Science (2016): Impact factor 19.304
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 14.38
Web of Science (2015): Impact factor 17.184
Web of Science (2015): Indexed yes
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BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 14.96
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ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 14.01
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Atomic structure and energetics of screw dislocations in copper

General information
State: Published
Organisations: Department of Physics, Risø National Laboratory
Contributors: Rasmussen, T., Jacobsen, K. W., Leffers, T., Pedersen, O.
Pages: 544
Publication date: 1997
Peer-reviewed: Yes

Publication information
Journal: Materials Science and Engineering A
Volume: A234
ISSN (Print): 0921-5093
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.76 SJR 1.694 SNIP 1.943
Web of Science (2017): Impact factor 3.414
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.669 SNIP 1.913
Web of Science (2016): Impact factor 3.094
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.01 SJR 1.742 SNIP 1.858
Web of Science (2015): Impact factor 2.647
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.32 SJR 2.235 SNIP 2.546
Web of Science (2014): Impact factor 2.567
Web of Science (2014): Indexed yes
Atomistic Determination of Cross-Slip Pathway and Energetics
The mechanism for cross slip of a screw dislocation in Cu is determined by atomistic simulations that only presume the initial and final states of the process. The dissociated dislocation constricts in the primary plane and redissociates into the cross-slip plane while still partly in the primary plane. The transition state and activation energy for cross slip as well as the energies of the involved dislocation constrictions are determined. One constriction has a negative energy compared to parallel partials. The energy vs splitting width for recombination of parallel partials into a perfect dislocation is determined. The breakdown of linear elasticity theory for small splitting widths is studied. [S0031-9007(97)04444-X].

General information
Comment on "Cs-Induced Relaxation of the Cu(110) Surface"
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Original language: English
Keywords: ENERGY ELECTRON-DIFFRACTION, CU
Electronic versions:
AC.pdf
DOIs:
10.1103/PhysRevLett.78.158
URLs:
http://link.aps.org/doi/10.1103/PhysRevLett.78.158

**Bibliographical note**
Source: orbit
Conductance eigenchannels in nanocontacts
The electronic conductance of metal nanocontacts is analyzed in terms of eigenchannels for the transmission. The transmission through individual eigenchannels is calculated numerically for realistic models of gold point contacts based on molecular-dynamics simulation of the elongation of a contact. The conductance as a function of contact elongation exhibits a step structure. For the smallest contact areas of one or a few atom diameters, the conductance is typically quantized, and a specific number of almost open eigenchannels can be ascribed. For larger contact areas the scattering leads to partly open channels, but plateaus in the conductance can still be present. We also show that the finite stiffness of the experimental setup can significantly affect the step structure of the conductance curves.
Heteroepitaxial subsurface growth mode resulting in interlayer mixing

A subsurface growth mode which results in interlayer mixing has been revealed from an interplay between scanning tunneling microscopy and ab initio total-energy calculations for the growth of Pd on Cu(110) and Ag(110) surfaces. On Cu(110), the Pd initially alloys into the surface layer forming ordered linear -Pd-Cu- chains. As the coverage is increased, the -Pd-Cu- chains remain at the same level, but become covered, partly by Cu atoms expelled during alloying, partly by substrate material supplied from steps and terraces. This results in a very rough surface morphology, even at relatively low Pd coverages. Similar structures were observed on Ag(110). The observed growth mode is expected to apply to other heteroepitaxial systems as well.
Ratings:

BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Impact factor 3.813
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Impact factor 3.836
Web of Science (2016): Indexed yes
Scopus rating (2015): CiteScore 2.8 SJR 2.377 SNIP 1.13
Web of Science (2015): Impact factor 3.718
Web of Science (2015): Indexed yes
Scopus rating (2014): CiteScore 3.3 SJR 2.762 SNIP 1.316
Web of Science (2014): Impact factor 3.736
Web of Science (2014): Indexed yes
Scopus rating (2013): CiteScore 3.55 SJR 2.813 SNIP 1.326
Web of Science (2013): Impact factor 3.664
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): CiteScore 3.57 SJR 3.173 SNIP 1.378
Web of Science (2012): Impact factor 3.767
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): CiteScore 3.61 SJR 3.326 SNIP 1.423
Web of Science (2011): Impact factor 3.691
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 3.318 SNIP 1.447
Web of Science (2010): Impact factor 3.774
Web of Science (2010): Indexed yes
Web of Science (2009): Indexed yes
Scopus rating (2008): SJR 2.923 SNIP 1.516
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.892 SNIP 1.588
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.62 SNIP 1.468
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.126 SNIP 1.156
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.012 SNIP 1.103
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.184 SNIP 1.179
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.856 SNIP 1.841
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 3.132 SNIP 1.727
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 2.84 SNIP 1.603
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 2.789 SNIP 1.541

Original language: English
Keywords: SURFACE, AG(110), CU-NI, AU, ALLOYS, SCANNING-TUNNELING-MICROSCOPY
Phase diagrams for surface alloys

We discuss surface alloy phases and their stability based on surface phase diagrams constructed from the surface energy as a function of the surface composition. We show that in the simplest cases of pseudomorphic overlayers there are four generic classes of systems, characterized by the sign of the heat of segregation from the bulk and the sign of the excess interactions between the atoms in the surface (the surface mixing energy). We also consider the more complicated cases with ordered surface phases, nonpseudomorphic overlayers, second layer segregation, and multilayers. The discussion is based on density-functional calculations using the coherent-potential approximation and on effective-medium theory. We give self-consistent density-functional results for the segregation energy and surface mixing energy for all combinations of the transition and noble metals. Finally we discuss in detail the cases Ag/Cu(100), Pt/Cu(111), Ag/Pt(111), Co/Cu(111), Fe/Cu(111), and Pd/Cu(110) in connection with available experimental results.
Scopus rating (2015): CiteScore 2.8 SJR 2.377 SNIP 1.13
Web of Science (2015): Impact factor 3.718
Web of Science (2015): Indexed yes
Scopus rating (2014): CiteScore 3.3 SJR 2.762 SNIP 1.316
Web of Science (2014): Impact factor 3.736
Web of Science (2014): Indexed yes
Scopus rating (2013): CiteScore 3.55 SJR 2.813 SNIP 1.326
Web of Science (2013): Impact factor 3.664
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): CiteScore 3.57 SJR 3.173 SNIP 1.378
Web of Science (2012): Impact factor 3.767
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): CiteScore 3.61 SJR 3.326 SNIP 1.423
Web of Science (2011): Impact factor 3.691
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 3.318 SNIP 1.447
Web of Science (2010): Impact factor 3.774
Web of Science (2010): Indexed yes
Web of Science (2009): Indexed yes
Scopus rating (2008): SJR 2.923 SNIP 1.516
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.892 SNIP 1.588
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.62 SNIP 1.468
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.126 SNIP 1.156
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.012 SNIP 1.103
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.184 SNIP 1.179
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.856 SNIP 1.841
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 3.132 SNIP 1.727
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 2.84 SNIP 1.603
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 2.789 SNIP 1.541
Original language: English
Keywords: ELECTRONIC-STRUCTURE, METAL-METAL INTERFACES, THIN-FILMS, CU-NI, INITIAL GROWTH, IMMISCIBLE METALS, AU, SEGREGATION, CU(100), SCANNING-TUNNELING-MICROSCOPY
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Copyright (1997) by the American Physical Society.
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Research output: Research - peer-review › Journal article – Annual report year: 1997
Rate Theory for Correlated Processes: Double Jumps in Adatom Diffusion

We study the rate of activated motion over multiple barriers, in particular the correlated double jump of an adatom diffusing on a missing-row reconstructed platinum (110) surface. We develop a transition path theory, showing that the activation energy is given by the minimum-energy trajectory which succeeds in the double jump. We explicitly calculate this trajectory within an effective-medium molecular dynamics simulation. A cusp in the acceptance region leads to a root $T$ prefactor for the activated rate of double jumps. Theory and numerical results agree.

General information
State: Published
Organisations: Theoretical Atomic-scale Physics, Department of Physics, Cornell University
Contributors: Jacobsen, J., Jacobsen, K. W., Sethna, J.
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Peer-reviewed: Yes

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Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 7.58 SJR 3.622 SNIP 2.464
Web of Science (2017): Impact factor 8.839
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.33 SJR 4.196 SNIP 2.61
Web of Science (2016): Impact factor 8.462
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.76 SJR 4.656 SNIP 2.538
Web of Science (2015): Impact factor 7.645
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.62 SJR 5.232 SNIP 2.71
Web of Science (2014): Impact factor 7.512
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 7.46 SJR 5.675 SNIP 2.781
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 7.19 SJR 6.292 SNIP 2.867
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 7.02 SJR 6.314 SNIP 2.905
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 6.45 SNIP 2.757
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 6.325 SNIP 2.947
Scattering and conductance quantization in three-dimensional metal nanocontacts

The transmission through three-dimensional nanocontacts is calculated in the presence of localized scattering centers and boundary scattering using a coupled-channel recursion method. Simple confining potentials are used to investigate how robust the observation of quantized conductance is with respect to the scattering. We find that the quantum features are quite stable: the scattering by a localized scatterer will selectively smear and downshift certain quantum steps depending on the position of the scatterer, but the remaining steps will still be at integer positions. The effect of scattering by surface corrugation depends on the length scale of the corrugation. In some cases a significant downshift of the steps without accompanying smearing is observed. In general, we find that even in the cases where scattering shifts the quantum steps the quantization of the motion perpendicular to the contacts remains intact. Non-integer steps can therefore also be a signature of quantized conductance.
Simulations of the atomic structure, energetics, and cross slip of screw dislocations in copper

Using nanoscale atomistic simulations it has been possible to address the problem of cross slip of a dissociated screw dislocation in an fcc metal (Cu) by a method not suffering from the limitations imposed by elasticity theory. The focus has been on different dislocation configurations relevant for cross slip via the Friedel-Escaig (FE) cross-slip mechanism. The stress free cross-slip activation energy and activation length for this mechanism are determined. We show that the two constrictions necessary for cross slip in the FE cross-slip mechanism are not equivalent and that a dislocation configuration with just one of these constrictions is energetically favored over two parallel Shockley partials. The effect of having the dislocation perpendicular to a free surface is investigated. The results are in qualitative agreement with transmission electron microscopy experiments and predictions from linear-elasticity theory showing recombination or repulsion of the partials near the free surface. Such recombination at the free surface might be important in the context of cross slip because it allows the creation of the above-mentioned energetically favorable constriction alone. In addition we observe a strong preference for the partials to be in a glide plane parallel to the surface step. We have performed simulations of two screw dislocations of opposite signs, one simulation showing surface nucleated cross slip leading to subsequent annihilation of the two dislocations. It was possible to monitor the annihilation process, thereby determining the detailed dislocation reactions during annihilation.
Anisotropic corner diffusion as origin for dendritic growth on hexagonal substrates

Ag aggregation on Ag(111), Pt(111), and 1 ML Ag pseudomorphically grown on Pt(111), has been studied with variable temperature STM. These systems all have in common that dendritic patterns with trigonal symmetry rather than randomly ramified aggregates, which would be expected for a simple hit and stick mechanism, form. Dendrites are characterized by preferential growth in the \([<11\overline{2}>]\)-directions, i.e., perpendicular to A-steps. The key process for their formation has been found to be diffusion of one-fold corner atoms towards neighboring steps. Calculations with the effective medium theory show that this relaxation is highly asymmetric with respect to the two different kinds of close-packed steps. It leads to dendritic growth as verified by kinetic Monte-Carlo simulations which agree well with experiment.
Apparent Barrier Height in Scanning Tunneling Microscopy Revisited

The apparent barrier height $\phi_{ap}$, that is, the rate of change of the logarithm of the conductance with tip-sample separation in a scanning tunneling microscope (STM), has been measured for Ni, Pt, and Au single crystal surfaces. The results show that $\phi_{ap}$ is constant until point contact is reached rather than decreasing at small tunneling gap distances, as previously reported. The findings for $\phi_{ap}$ can be accounted for theoretically by including the relaxations of the tip-surface junction in an STM due to the strong adhesive forces at close proximity. These relaxation effects are shown also to be generally relevant under imaging conditions at metal surfaces.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Aarhus University
Contributors: Olesen, L., Brandbyge, M., Sørensen, M. R., Jacobsen, K. W., Lægsgaard, E., Stensgaard, I., Besenbacher, F.
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Web of Science (2018): Indexed yes
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Scopus rating (2017): CiteScore 7.58 SJR 3.622 SNIP 2.464
Web of Science (2017): Impact factor 8.839
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.33 SJR 4.196 SNIP 2.61
Web of Science (2016): Impact factor 8.462
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
A semi-empirical effective medium theory for metals and alloys
A detailed derivation of the simplest form of the effective medium theory for bonding in metallic systems is presented, and parameters for the fcc metals Ni, Pd, Pt, Cu, Ag and Au are given. The derivation of parameters is discussed in detail to show how new parameterizations can be made. The method and the parameterization is tested for a number of surface and bulk problems. In particular we present calculations of the energetics of metal atoms deposited on metal surfaces. The calculated energies include heats of adsorption, energies of overlayers, both pseudomorphic and relaxed, as well as energies of atoms alloyed into the first surface layer.

General information
State: Published
Organisations: Department of Physics
Contributors: Jacobsen, K. W., Stoltze, P., Nørskov, J. K.
Pages: 394-402
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Peer-reviewed: Yes

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Journal: Surface Science
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Issue number: 2
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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.87 SJR 0.81 SNIP 0.759
Web of Science (2017): Impact factor 1.997
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.85 SJR 0.746 SNIP 0.834
Web of Science (2016): Impact factor 2.062
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.85 SJR 0.747 SNIP 0.804
Web of Science (2015): Impact factor 1.931
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.81 SJR 0.818 SNIP 0.864
Web of Science (2014): Impact factor 1.925
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.72 SJR 0.829 SNIP 0.781
Web of Science (2013): Impact factor 1.87
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.91 SJR 1.096 SNIP 0.878
Web of Science (2012): Impact factor 1.838
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.88 SJR 1.076 SNIP 0.906
Web of Science (2011): Impact factor 1.994
Density functional theory study of self-diffusion on the (111) surfaces of Ni, Pd, Pt, Cu, Ag and Au

General information
State: Published
Organisations: Department of Physics
Pages: 173
Publication date: 1996
Peer-reviewed: Yes

Publication information
Journal: Springer Series on Solid State Physics, Ed. A. Okiji
Volume: 121
Original language: English
Source: orbit
Source-ID: 165600
Research output: Research - peer-review; Journal article – Annual report year: 1996

Homoepitaxial Growth of Pt on Pt(100)-hex: Effects of Strongly Anisotropic Diffusion and Finite Island Sizes
Nucleation and growth of Pt on the reconstructed Pt(100)-hex surface was studied by scanning tunneling microscopy. A detailed autocorrelation analysis of island positions reveals direct evidence for strongly anisotropic diffusion, and from the island size distribution, which obeys a simple scaling relation, we conclude that the mobility of dimers is negligible. Finally, kinetic Monte Carlo simulations, incorporating anisotropy in diffusion and finite island sizes, yield new insight into how these two factors affect the island size distribution and the scaling behavior of island density with temperature and
deposition rate.

**General information**
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Aarhus University
Contributors: Linderoth, T., Mortensen, J. J., Jacobsen, K. W., Lægsgaard, E., Stensgaard, I., Besenbacher, F.
Pages: 87-90
Publication date: 1996
Peer-reviewed: Yes

**Publication information**
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Volume: 77
Issue number: 1
ISSN (Print): 0031-9007
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 7.58 SJR 3.622 SNIP 2.464
Web of Science (2017): Impact factor 8.839
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.33 SJR 4.196 SNIP 2.61
Web of Science (2016): Impact factor 8.462
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.76 SJR 4.656 SNIP 2.538
Web of Science (2015): Impact factor 7.645
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.62 SJR 5.232 SNIP 2.71
Web of Science (2014): Impact factor 7.512
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 7.46 SJR 5.675 SNIP 2.781
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 7.19 SJR 6.292 SNIP 2.867
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 7.02 SJR 6.314 SNIP 2.905
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 6.45 SNIP 2.757
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 6.325 SNIP 2.947
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 6.194 SNIP 2.837
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 5.95 SNIP 2.738
Island shapes in homoepitaxial growth of Pt(111)

We present a kinetic model for the homoepitaxial growth of Pt(111) capable of reproducing the experimentally observed compact island shapes in a set of kinetic Monte-Carlo simulations. We propose that an anomaly in the binding of single atoms to the two types of close packed steps causes the appearance of triangular islands around 400 K. The anomaly is that the single atoms bind the strongest to the more stable close packed step. We argue, that this cannot be the cage for longer rows of atoms attached to the steps, and assuming that dimers bind the strongest to the less stable close packed step, we show this causes the appearance of triangular islands of the opposite orientation around 650 K.

General information
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Organisations: Department of Physics
Contributors: Jacobsen, J., Jacobsen, K. W., Nørskov, J. K.
Pages: 37-44
Publication date: 1996
Peer-reviewed: Yes

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Journal: Surface Science
Volume: 359
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ISSN (Print): 0039-6028
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.87 SJR 0.81 SNIP 0.759
Web of Science (2017): Impact factor 1.997
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.85 SJR 0.746 SNIP 0.834
Web of Science (2016): Impact factor 2.062
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.85 SJR 0.747 SNIP 0.804
Web of Science (2015): Impact factor 1.931
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.81 SJR 0.818 SNIP 0.864
Web of Science (2014): Impact factor 1.925
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.72 SJR 0.829 SNIP 0.781
Web of Science (2013): Impact factor 1.87
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.91 SJR 1.096 SNIP 0.878
Web of Science (2012): Impact factor 1.838
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.88 SJR 1.076 SNIP 0.906
Web of Science (2011): Impact factor 1.994
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.228 SNIP 0.858
Web of Science (2010): Impact factor 2.011
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.129 SNIP 0.896
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.215 SNIP 0.838
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.134 SNIP 0.856
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.287 SNIP 0.947
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.46 SNIP 1.044
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.57 SNIP 1.082
Scopus rating (2003): SJR 1.718 SNIP 1.09
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.401 SNIP 1.049
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.812 SNIP 1.041
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.979 SNIP 0.954
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.752 SNIP 0.974
Original language: English
Mechanical deformation of nanocrystalline materials

General information
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Organisations: Department of Physics
Contributors: Schiøtz, J., Rasmussen, T., Nielsen, O. H., Jacobsen, K. W.
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Peer-reviewed: Yes

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ISSN (Print): 0950-0839
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.12 SJR 0.58 SNIP 0.584
Web of Science (2017): Impact factor 1.194
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.1 SJR 0.703 SNIP 0.665
Web of Science (2016): Impact factor 0.941
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.08 SJR 0.718 SNIP 0.672
Web of Science (2015): Impact factor 0.918
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.24 SJR 0.89 SNIP 0.758
Web of Science (2014): Impact factor 1.087
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.31 SJR 0.978 SNIP 0.934
Web of Science (2013): Impact factor 1.268
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.17 SJR 0.814 SNIP 0.938
Web of Science (2012): Impact factor 1.156
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 1.31 SJR 0.92 SNIP 0.98
Web of Science (2011): Impact factor 1.241
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.195 SNIP 0.858
Web of Science (2010): Impact factor 1.262
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.377 SNIP 0.927
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.681 SNIP 0.953
Simulations of atomic-scale sliding friction

Simulation studies of atomic-scale sliding friction have been performed for a number of tip-surface and surface-surface contacts consisting of copper atoms. Both geometrically very simple tip-surface structures and more realistic interface necks formed by simulated annealing have been studied. Kinetic friction is observed to be caused by atomic-scale Stick and slip which occurs by nucleation and subsequent motion of dislocations preferably between close-packed (111) planes. Stick and slip seems to occur in different situations. For single crystalline contacts without grain boundaries at the interface the stick and slip process is clearly observed for a large number of contact areas, normal loads, and sliding velocities. If the tip and substrate crystal orientations are different so that a mismatch exists in the interface, the stick and slip process is more fragile. It is then caused by local pinning of atoms near the boundary of the interface and is therefore more easily observed for smaller contacts. Depending on crystal orientation and load, frictional wear can also be seen in the simulations. In particular, for the annealed interface-necks which model contacts created by scanning tunneling microscope/atomic force microscope tip indentations the sliding process involves breaking contacts leaving tip material behind on the substrate.

General information

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Organisations: Department of Physics, Theoretical Atomic-scale Physics
Contributors: Sørensen, M. R., Jacobsen, K. W., Stoltze, P.
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Peer-reviewed: Yes

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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Impact factor 3.813
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Impact factor 3.836
Web of Science (2016): Indexed yes
Scopus rating (2015): CiteScore 2.8 SJR 2.377 SNIP 1.13
Web of Science (2015): Impact factor 3.718
Web of Science (2015): Indexed yes
Scopus rating (2014): CiteScore 3.3 SJR 2.762 SNIP 1.316
Web of Science (2014): Impact factor 3.736
Thermal Diffusion Processes in Metal-Tip-Surface Interactions: Contact Formation and Adatom Mobility

We have carried out computer simulations to identify and characterize various thermally activated atomic scale processes that can play an important role in room temperature experiments where a metal tip is brought close to a metal surface. We find that contact formation between the tip and the surface can occur by a sequence of atomic hop and exchange processes which become active on a millisecond time scale when the tip is about 3-5 Angstrom from the surface. Adatoms
on the surface are stabilized by the presence of the tip and energy barriers for diffusion processes in the region under the tip are reduced. This can cause adatoms to follow the tip as it is moved over the surface.
Atomic-Scale Determination of Misfit Dislocation Loops at Metal-Metal Interfaces

The growth of one monolayer of Au on Ni(111) is shown to lead to an ordered array of misfit dislocation loops in the underlying Ni(111) surface. The signature of these loops is observed by scanning tunneling microscopy, and atomistic simulations are used to relate the observed surface structure to that of the buried interface. The new interface structure is different from normal misfit dislocation structures in three respects: (i) it forms already during growth of a single Au monolayer, (ii) it forms in the substrate and not in the overlayer, and (iii) it is controlled by the interface energy rather than by the strain in the two phases.

General information
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Organisations: Department of Physics, Theoretical Atomic-scale Physics, Technical University of Denmark
Pages: 489-492
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 7.58 SJR 3.622 SNIP 2.464
Web of Science (2017): Impact factor 8.839
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.33 SJR 4.196 SNIP 2.61
Web of Science (2016): Impact factor 8.462
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.76 SJR 4.656 SNIP 2.538
Web of Science (2015): Impact factor 7.645
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.62 SJR 5.232 SNIP 2.71
Web of Science (2014): Impact factor 7.512
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 7.46 SJR 5.675 SNIP 2.781
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 7.19 SJR 6.292 SNIP 2.867
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 7.02 SJR 6.314 SNIP 2.905
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 6.45 SNIP 2.757
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 6.325 SNIP 2.947
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 6.194 SNIP 2.837
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 5.95 SNIP 2.738
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 4.781 SNIP 2.443
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 4.082 SNIP 2.101
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 3.847 SNIP 2.122
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 4.661 SNIP 2.651
Web of Science (2003): Indexed yes
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 5.884 SNIP 3.375
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 5.618 SNIP 3.135
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 5.771 SNIP 2.941
Original language: English
Effect of strain on surface diffusion and nucleation

The influence of strain on diffusion and nucleation has been studied by means of scanning tunneling microscopy and effective-medium theory for Ag self-diffusion on strained and unstrained (111) surfaces. Experimentally, the diffusion barrier is observed to be substantially lower on a pseudomorphic Ag monolayer on Pt(111), 60 meV, compared to that on Ag(111), 97 meV. The calculations show that this strong effect is due to the 4.2% compressive strain of the Ag monolayer on Pt. It is shown that in general isotropic two-dimensional strain as well as its relief via dislocations have a drastic effect on surface diffusion and nucleation in heteroepitaxy and are thus of significance for the film morphology in the kinetic growth regime.
A set of density-functional calculations for clean and O-covered Al(111) are presented. At low O coverages the potential energy surface (PES) of chemisorbed O is investigated. The PES indicates large barriers (0.8 eV) against O diffusion and a large corrugation of the equilibrium O height over the Al(111) while only a moderate energy gain (5 eV per atom) is found upon Oz dissociation over the surface. The possible existence of "hot" O adatoms after O-2 dissociation is discussed on the basis of the presented PES and existing dynamical simulations on model potentials. At high O coverages an attractive O-O interaction is identified together with an enhancement in the dipole moment induced per O atom. Finally, Tersoff-Hamann-type scanning tunneling microscopy (STM) topographs are derived based on the calculated one-electron wave functions and spectra. For the clean Al(111) a theoretical STM height corrugation compatible with the experimentally observed one is obtained if the tunneling conductance is assumed dominated by contributions from orbitals of atomic p character centered on the tip. For the O-covered Al(111) the theoretical topographs agree well with the observed ones.
Island Shape-Induced Transition from 2D to 3D Growth for Pt/Pt(111)

We present a kinetic Monte Carlo simulation of the growth of Pt on Pt(111) capable of describing the experimentally observed temperature dependence of the island shapes and the growth mode. We show that the transition from a 2D growth mode at low temperatures to a 3D mode at higher temperatures is closely related to the disappearance of kink sites and the appearance of the triangular islands observed in the 3D growth regime.
Nature of Dislocations in Silicon

Interaction between two partial 90 degrees edge dislocations is studied with atomic-scale simulations using the effective-medium tight-binding method. A large separation between the two dislocations (up to 30 Angstrom), comparable to experimental values, is achieved with a solution of the tight-binding Hamiltonian that scales linearly with the number of atoms. The partial edge dislocation is found to be very accurately described by the Peierls-Nabarro dislocation model, with generalized stacking-fault restoring forces, as reflected both in the interaction energy and in the displacement field. An asymmetric core reconstruction provides fourfold coordination, making Si behave elastically down to atomic distances.

General information
State: Published
Organisations: Theoretical Atomic-scale Physics, Department of Physics, Ames Laboratory
Contributors: Hansen, L. B., Stokbro, K., Lundqvist, B., Jacobsen, K. W., Deaven, D. M.
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Peer-reviewed: Yes

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Web of Science (2018): Indexed yes
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Web of Science (2017): Impact factor 8.839
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.33 SJR 4.196 SNIP 2.61
Web of Science (2016): Impact factor 8.462
Web of Science (2016): Indexed yes
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Scopus rating (2015): CiteScore 5.76 SJR 4.656 SNIP 2.538
Web of Science (2015): Impact factor 7.645
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.62 SJR 5.232 SNIP 2.71
Web of Science (2014): Impact factor 7.512
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 7.46 SJR 5.675 SNIP 2.781
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 7.19 SJR 6.292 SNIP 2.867
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 7.02 SJR 6.314 SNIP 2.905
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 6.45 SNIP 2.757
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Quantized conductance in an atom-sized point-contact - Reply
A Reply to the Comment by J. M. Krans et al.

General information
State: Published
Organisations: Experimental Surface and Nanomaterials Physics, Department of Physics, Theoretical Atomic-scale Physics, Aarhus University
Pages: 2147-2147
Publication date: 1995
Peer-reviewed: Yes

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Volume: 74
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ISSN (Print): 0031-9007
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Quantized conductance in atom-sized wires between two metals
We present experimental and theoretical results for the conductance and mechanical properties of atom-sized wires between two metals. The experimental part is based on measurements with a scanning tunneling microscope (STM) where a point contact is created by indenting the tip into a gold surface. When the tip is retracted, a 10-20 Angstrom long nanowire is formed. Our measurements of the conductance of nanowires show clear signs of a quantization in units of $2e^2/h$. The scatter around the integer values increases considerably with the number of quanta, and typically it is not possible to observe more than up to four quanta in these experiments. A detailed discussion is given of the statistical methods used in the analysis of the experimental data. The theoretical part of the paper addresses some questions posed by the experiment: Why can conductance quantization be observed, what is the origin of the scatter in the experimental data, and what is the origin of the scaling of the scattering with the number of conductance quanta? The theoretical discussion is based on a free-electron-like model where scattering from the boundary of the nanowire is included. The configurations of the nanowires are deduced from molecular dynamics simulations, which also give information about the mechanical properties of the system. We show that such a model can account semiquantitatively for several of the observed effects. One of the main conclusions of the theoretical analysis is that, due to the plastic deformation of the nanowires formed by the STM, the typical length scale of the variations in the shape of the boundary is not an atomic radius but rather a size times that value. This is the reason why scattering is sufficiently small to make conductance quantization observable by STM.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Theoretical Atomic-scale Physics, Aarhus University
Pages: 8499-8514
Publication date: 1995
Peer-reviewed: Yes

Publication information
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Volume: 52
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Impact factor 3.813
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Impact factor 3.836
Web of Science (2016): Indexed yes
Scopus rating (2015): CiteScore 2.8 SJR 2.377 SNIP 1.13
Web of Science (2015): Impact factor 3.718
Web of Science (2015): Indexed yes
Scopus rating (2014): CiteScore 3.3 SJR 2.762 SNIP 1.316
Surface stress, surface elasticity, and the size effect in surface segregation

Surface stress and surface elasticity of low-index fcc surfaces have been studied using effective-medium theory potentials. In addition to total-energy calculations giving stress components and elastic data for the surface as a whole, the use of artificial atoms with modified size allows us to probe the stress and elasticity of individual layers. This method of artificial atoms provides a direct way to study the contribution of atomic size to segregation in alloys as well as the driving force of reconstructions driven by surface stress. As an example, we give a qualitative explanation of the face-dependent segregation of Pt-Ni alloys. We also compare results of these atomic-scale calculations with continuum elasticity.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Vienna University of Technology
Pages: 10937-10946
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Peer-reviewed: Yes

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Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Impact factor 3.813
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Impact factor 3.836
Web of Science (2016): Indexed yes
Scopus rating (2015): CiteScore 2.8 SJR 2.377 SNIP 1.13
Web of Science (2015): Impact factor 3.718
Web of Science (2015): Indexed yes
Scopus rating (2014): CiteScore 3.3 SJR 2.762 SNIP 1.316
Web of Science (2014): Impact factor 3.736
Web of Science (2014): Indexed yes
Scopus rating (2013): CiteScore 3.55 SJR 2.813 SNIP 1.326
Web of Science (2013): Impact factor 3.664
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): CiteScore 3.57 SJR 3.173 SNIP 1.378
Web of Science (2012): Impact factor 3.767
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): CiteScore 3.61 SJR 3.326 SNIP 1.423
Web of Science (2011): Impact factor 3.691
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 3.318 SNIP 1.447
Web of Science (2010): Impact factor 3.774
Web of Science (2010): Indexed yes
Web of Science (2009): Indexed yes
Scopus rating (2008): SJR 2.923 SNIP 1.516
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.892 SNIP 1.588
Effective-medium tight-binding model for silicon

A method for calculating the total energy of Si systems, which is based on the effective-medium-theory concept of a reference system, is presented. Instead of calculating the energy of an atom in the system of interest, a reference system is introduced where the local surroundings are similar. The energy of the reference system can be calculated self-consistently once and for all while the energy difference to the reference system can be obtained approximately. We propose to calculate it using the tight-binding linear-muffin-tin-orbital scheme with the atomic-sphere approximation (ASA) for the potential, and by using the ASA with charge-conserving spheres we are able to treat open systems without introducing empty spheres. All steps in the calculational method are ab initio in the sense that all quantities entering are calculated from first principles without any fitting to experiment. A complete and detailed description of the method is given together with test calculations of the energies of phonons, elastic constants, different structures, surfaces, and surface reconstructions. We compare the results to calculations using an empirical tight-binding scheme.
Multidimensional Potential Energy Surface for H₂ Dissociation over Cu(111)

We present ab initio density functional calculations within the generalized gradient approximation for H₂ dissociating over Cu(111). The minimum barrier for dissociation is 0.5 eV and shows large corrugation within the unit cell and a strong dependence on the molecular orientation. Dissociation is predicted to depend strongly on translational, vibrational, and rotational degrees of freedom in accordance with experiment. We show that even for a noble metal, the d electrons are important for the molecule-surface interaction.
Quantized conductance in an atom-sized point contact

We present direct measurements at room temperature of the conductance of a point contact between a scanning tunneling microscope tip and Ni, Cu, and Pt surfaces. As the contact is stretched the conductance jumps in units of $2e^2/h$. Atomistic simulations of the stretch of the contact combined with calculations of the conductance using the Landauer formula show that the observed behavior is due to the quantization of the transverse electron motion in a contact which contains between one and ten atoms.
Self-consistent electronic structure and segregation profiles of the Cu-Ni (001) random-alloy surface

We have calculated the electronic structure and segregation profiles of the (001) surface of random Cu-Ni alloys with varying bulk concentrations by means of the coherent potential approximation and the linear muffin-tin-orbitals method. Exchange and correlation were included within the local-density approximation. Temperature effects were accounted for by means of the cluster-variation method and, for comparison, by mean-field theory. The necessary interaction parameters were calculated by the Connolly-Williams method generalized to the case of a surface of a random alloy. We find the segregation profiles to be oscillatory with a strong preference for Cu to segregate towards the surface of the alloy.

General information

State: Published
Organisations: Theoretical Atomic-scale Physics, Department of Physics, Uppsala University, Moscow Institute for Steel and Alloys
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Peer-reviewed: Yes

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BFI (2018): BFI-level 1
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Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Impact factor 3.836
Web of Science (2016): Indexed yes
Scopus rating (2015): CiteScore 2.8 SJR 2.377 SNIP 1.13
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Web of Science (2015): Indexed yes
Scopus rating (2014): CiteScore 3.3 SJR 2.762 SNIP 1.316
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Scopus rating (2012): CiteScore 3.57 SJR 3.173 SNIP 1.378
Web of Science (2012): Impact factor 3.767
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): CiteScore 3.61 SJR 3.326 SNIP 1.423
Web of Science (2011): Impact factor 3.691
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 3.318 SNIP 1.447
Web of Science (2010): Impact factor 3.774
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Web of Science (2009): Indexed yes
Scopus rating (2008): SJR 2.923 SNIP 1.516
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Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.62 SNIP 1.468
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.126 SNIP 1.156
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.012 SNIP 1.103
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.184 SNIP 1.179
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.856 SNIP 1.841
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 3.132 SNIP 1.727
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 2.84 SNIP 1.603
Web of Science (2000): Indexed yes
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Initial growth of Au on Ni(110): Surface alloying of immiscible metals

Atomic resolution scanning tunneling microscopy of Au deposited on Ni(110) shows that even though Au is completely insoluble in bulk Ni, it replaces Ni in the first surface layer forming a surface Au-Ni alloy and the squeezed out Ni atoms agglomerate in Ni islands on the surface. This picture is supported by total energy calculations within the effective-medium theory, which also provide a detailed understanding of this surprising phenomenon.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Aarhus University, Technical University of Denmark
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Peer-reviewed: Yes

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Web of Science (2017): Impact factor 8.839
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.33 SJR 4.196 SNIP 2.61
Web of Science (2016): Impact factor 8.462
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.76 SJR 4.656 SNIP 2.538
Web of Science (2015): Impact factor 7.645
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.62 SJR 5.232 SNIP 2.71
Web of Science (2014): Impact factor 7.512
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 7.46 SJR 5.675 SNIP 2.781
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 7.19 SJR 6.292 SNIP 2.867
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 7.02 SJR 6.314 SNIP 2.905
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Role of nonlocal exchange correlation in activated adsorption
The barrier for dissociative adsorption of H-2 on Al(110) has been calculated within the generalized gradient approximation. A pronounced increase of the barrier height is found compared with what is calculated in the local density approximation (LDA). The apparent LDA underestimation of the barrier height is shown to be intimately linked with the LDA underbinding of core electrons and we suggest it to be a general phenomenon not limited to the particular nonlocal exchange-correlation approximation used or the particular system studied.

General information
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Organisations: Department of Physics, Theoretical Atomic-scale Physics
Contributors: Hammer, B., Jacobsen, K. W., Nørskov, J. K.
Pages: 3971-3974
Publication date: 1993
Peer-reviewed: Yes

Publication information
Journal: Physical Review Letters
Volume: 70
Issue number: 25
Ab initio potential for solids
A total-energy theory for a solid is presented. It is based on density-functional theory and consists of a succession of approximations. At the most accurate level, the theory consists of a systematic derivation of an ansatz for the electron density which is best suited for the Harris functional. At the most approximate level, the theory is equivalent to the usual effective-medium theory. At all levels of approximation, every term in the total-energy expression is calculated ab initio, that is, without any fitting to experiment or to other calculations. Every step in the approximation procedure can thus be tested independently. The theory is applied to calculations of the surface energies and vacancy formation energy of Al. At the most accurate level, the theory gives results that are in almost complete agreement with self-consistent calculations. At the more approximate, but also computationally much less demanding, level, the theory gives results that are still in excellent agreement with the self-consistent results.
Dissociation path for H2 on Al(110)

The minimum energy path is calculated for an H2 molecule dissociating on an Al(110) surface within local density functional theory. The properties of the potential energy surface along the five H2 ionic coordinates perpendicular to the reaction path are also determined and shown to be essential for an understanding of the dissociation dynamics.
Theory of alkali-metal-induced reconstructions of fcc(100) surfaces

Calculations of missing-row reconstruction energies of the fcc(100) surfaces of the metals Al, Ni, Pd, Pt, Cu, Ag, and Au have been performed with the effective-medium theory with and without the presence of a potassium overlayer. It is shown that the tendency to reconstruct in the presence of adsorbed K is largest for Ag. This is in accordance with recent experiments indicating a potassium-induced missing-row reconstruction for Ag, but not for other metals. The tendency is shown to be related to the relatively low bulk modulus of silver. Differences from the well-known alkali-metal-induced reconstruction of fcc(110) surfaces are pointed out.

General information
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Organisations: Department of Physics
Contributors: Christensen, O. B., Jacobsen, K. W.
Pages: 6893-6898
Publication date: 1992
Peer-reviewed: Yes

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Journal: Physical Review B
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Ratings:
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Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Impact factor 3.813
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Impact factor 3.836
Cu cluster shell structure at elevated temperatures

Equilibrium structures of small (3–29)-atom Cu clusters are determined by simulated annealing, and finite-temperature ensembles are simulated by Monte Carlo techniques using the effective-medium theory for the energy calculation. Clusters with 8, 18, and 20 atoms are found to be particularly stable. The equilibrium geometrical structures are determined and found to be determined by a Jahn-Teller distortion, which is found to affect the geometry also at high temperatures. The “magic” clusters retain their large stability even at elevated temperatures.

General information
State: Published
Organisations: Department of Physics, University of Jyväskylä
Contributors: Christensen, O. B., Jacobsen, K. W., Nørskov, J. K., Manninen, M.
Pages: 2219-2222
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Peer-reviewed: Yes

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Issue number: 17
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Web of Science (2017): Impact factor 8.839
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.33 SJR 4.196 SNIP 2.61
Web of Science (2016): Impact factor 8.462
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.76 SJR 4.656 SNIP 2.538
Web of Science (2015): Impact factor 7.645
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.62 SJR 5.232 SNIP 2.71
Web of Science (2014): Impact factor 7.512
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 7.46 SJR 5.675 SNIP 2.781
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 7.19 SJR 6.292 SNIP 2.867
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 7.02 SJR 6.314 SNIP 2.905
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 6.45 SNIP 2.757
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Self-diffusion on copper surfaces
The diffusion paths and activation energies of a Cu adatom on Cu(100), Cu(111), and Cu(110) are studied using the effective-medium theory to calculate the energetics. For the (100) and (110) faces, diffusion via an exchange mechanism is found to be important. The transition state for these paths is stabilized by a direct covalent interaction as proposed by Feibelman. On the (111) face and for diffusion along the close-packed rows on the (110) surface, a simple hopping mechanism is found to be most favorable.

General information
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Organisations: Department of Physics, Theoretical Atomic-scale Physics, Technical University of Denmark
Pages: 6523-6526
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Peer-reviewed: Yes

Publication information
Journal: Physical Review B
Volume: 44
Issue number: 12
ISSN (Print): 2469-9950
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
Effective-medium calculations for hydrogen in Ni, Pd, and Pt

The effective-medium theory is applied to a study of the energetics of the hydrides of Ni, Pd, and Pt, stressing the properties of PdHθ for 0≤θ≤1. The calculated heat of solution and the heat of hydride formation for the three systems agree very well with experiment. We determine the favored structure for PdHθ by calculating the total energy and lattice expansion of different configurations. Vibrational frequencies and diffusion barriers of H in Pd are also treated. A simple and transparent physical picture of the hydrogen-metal interaction is developed. From the calculated energetics we make a model calculation of the phase diagram of hydrogen in palladium in qualitative agreement with experiment. On this basis we propose a new explanation of the peculiarities of the Pd-H system.
Oxygen chemisorption on Cu(110): A model for the c(6×2) structure

From an interplay between scanning tunneling microscopy, surface x-ray-diffraction experiments, and theoretical predictions, an unequivocal structural model for the Cu(110)-c(6×2)O surface reconstruction is derived with ten Cu atoms within the c(6×2) unit cell, two of which form a Cu superstructure. A general picture evolves in which the present as well as the Cu(110)-(2×1)O and the Cu(100)-(2√2 × √2 )R45°O reconstructions are stabilized by Cu-O-Cu chains directed along the [001] direction. The nucleation and growth of the c(6×2) structure occur preferentially at steps.

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Theoretical Atomic-scale Physics, Department of Physics, Aarhus University, University of Hamburg
Pages: 2027-2030
Publication date: 1990
Peer-reviewed: Yes

Publication information
Journal: Physical Review Letters
Volume: 65
Issue number: 16
Theory of the oxygen-induced restructuring of Cu(110) and Cu(100) surfaces
A model calculation based on the effective-medium theory of the oxygen-induced reconstruction of the (110) and (100) surfaces of Cu is presented. Equilibrium structures are calculated from a minimization of the total energy of the system. Missing-row-type reconstructions are found to be most stable in both cases, and an analysis is presented, showing what the driving force is behind these reconstructions.

General information
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Organisations: Theoretical Atomic-scale Physics, Department of Physics
Contributors: Jacobsen, K. W., Nørskov, J. K.
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Publication date: 1990
Peer-reviewed: Yes

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BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 7.58 SJR 3.622 SNIP 2.464
Web of Science (2017): Impact factor 8.839
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.33 SJR 4.196 SNIP 2.61
Web of Science (2016): Impact factor 8.462
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.76 SJR 4.656 SNIP 2.538
Web of Science (2015): Impact factor 7.645
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.62 SJR 5.232 SNIP 2.71
Web of Science (2014): Impact factor 7.512
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 7.46 SJR 5.675 SNIP 2.781
A discussion of the H-H interactions in a metal is given. Based on self-consistent total-energy calculations within the local-density approximation for H2 in a homogeneous electron gas, we show that metallic electrons make the H-H interaction more repulsive than in vacuum. Using effective-medium theory to calculate total energies we show the same tendency for the short-range part of the H-H interaction when two H atoms are squeezed into a single site in Pd or PdH. At longer range (of the order a lattice constant) there is an attractive, lattice-mediated H-H interaction. On the basis of the calculated energetics, the thermodynamical properties of various palladium hydrides are modeled.
Inelastic scattering in resonant tunneling

The exact resonant-tunneling transmission probability for an electron interacting with phonons is presented in the limit that the elastic coupling to the leads is independent of energy. The phonons produce transmission sidebands but do not affect the integrated transmission probability or the escape rate of the electron from the resonant site. In the Appendixes, we evaluate the Green function that appears in the expression for the transmission probability.
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Scopus rating (2012): CiteScore 3.57 SJR 3.173 SNIP 1.378
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Scopus rating (2011): CiteScore 3.61 SJR 3.326 SNIP 1.423
Web of Science (2011): Impact factor 3.691
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 3.318 SNIP 1.447
Web of Science (2010): Impact factor 3.774
Web of Science (2010): Indexed yes
Web of Science (2009): Indexed yes
Scopus rating (2008): SJR 2.923 SNIP 1.516
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.892 SNIP 1.588
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.62 SNIP 1.468
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.126 SNIP 1.156
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.012 SNIP 1.103
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.184 SNIP 1.179
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.856 SNIP 1.841
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 3.132 SNIP 1.727
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Scopus rating (2000): SJR 2.84 SNIP 1.603
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Projects:

An Analysis of Barrons Selv-organizing Controller
Lind, M., PhD Student, Department of Electrical Engineering
Jacobsen, K. W., Main Supervisor, Department of Physics
01/07/1970 → 04/10/1977
**Theoretical and Experimental determination of the stiffness and ultimate load of timber trusses**
Egerup, A., PhD Student, Department of Civil Engineering
Jacobsen, K. W., Main Supervisor, Department of Physics
01/08/1972 → 25/06/1975

**Computations of Harbour Oscillations by Ray Methods.**
Larsen, J. K., PhD Student, Department of Applied Mathematics and Computer Science
Jacobsen, K. W., Main Supervisor, Department of Physics
15/02/1974 → 29/06/1977

**A theoretical and experimental investigation of the LSA oscillator.**
Jeppesen, P., PhD Student, Department of Photonics Engineering
Jacobsen, K. W., Main Supervisor, Department of Physics
01/02/1967 → 31/07/1970

**Development of a Dynamic Model of a BWR Nuclear Power Plant.**
Nonbøl, E., PhD Student, Center for Nuclear Technologies
Jacobsen, K. W., Main Supervisor, Department of Physics
01/02/1973 → 06/10/1976

**Electron-Beam Pumped Luminescence and Laser Action in some II-VI Semiconducting Compounds.**
Hvam, J. M., PhD Student, Department of Photonics Engineering
Jacobsen, K. W., Main Supervisor, Department of Physics
01/02/1969 → 20/03/1972

**Theoretical studies of materials for water splitting**
Garijo del Río, E., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Thygesen, K. S., Supervisor, Department of Physics
Samfinansieret - Andet
01/08/2017 → 31/07/2020
Award relations: Theoretical studies of materials for water splitting

**Computational studies of two-dimension materials and heterosstructures**
Riis-Jensen, A. C., PhD Student, Department of Physics
Thygesen, K. S., Main Supervisor, Department of Physics
Jacobsen, K. W., Supervisor, Department of Physics
Institut stipendie (DTU)
15/07/2017 → 14/07/2020
Award relations: Computational studies of two-dimension materials and heterosstructures

**Chiral Magnetism from Mean Field Theory**
Torelli, D., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Christensen, N. B., Supervisor, Department of Physics
Olsen, T., Supervisor, Department of Physics
Olsen, T., Main Supervisor, Department of Physics
Forskningsrådsfinansiering
01/01/2017 → 31/12/2019
Award relations: Chiral Magnetism from Mean Field Theory
Project: PhD

**Nye funktionelle nanorør**
Strange, M., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Thygesen, K. S., Supervisor, Department of Physics
Schiotz, J., Examiner, Department of Physics
Puska, M. J., Examiner
Stokbro, K., Examiner, Department of Micro- and Nanotechnology

Programbevilling
15/06/2005 → 03/09/2008
Award relations: Nye funktionelle nanorør
Project: PhD

**Molekylære kontakters struktur, dynamik og transport**
Bækgaard, I. S. B., PhD Student, Department of Applied Mathematics and Computer Science
Jacobsen, K. W., Main Supervisor, Department of Physics
Thygesen, K. S., Supervisor, Department of Physics
Schiotz, J., Examiner, Department of Physics
Stokbro, K., Examiner, Department of Micro- and Nanotechnology
Todorov, T. N., Examiner

DTU-lønnet stipendie
01/03/2005 → 16/12/2009
Award relations: Molekylære kontakters struktur, dynamik og transport
Project: PhD

**Katalytiske egenskaber af nanopartikler på basis af elektronstrukturteori**
Moses, P. G., PhD Student, Department of Physics
Nørskov, J. K., Main Supervisor, Department of Physics
Jacobsen, K. W., Examiner, Department of Physics
Santen, R. A. V., Examiner
Schneider, W. F., Examiner

DTU-lønnet stipendie
01/01/2005 → 02/07/2008
Award relations: Katalytiske egenskaber af nanopartikler på basis af elektronstrukturteori
Project: PhD

**Materialedesign ved brug af tæthedsfunktionalteori og genetiske søgemetoder**
Fronczek-Munter, T. R., PhD Student, Department of Physics
Nørskov, J. K., Main Supervisor, Department of Physics
Christensen, C. H., Supervisor
Jacobsen, K. W., Examiner, Department of Physics
Hu, P., Examiner
Maier, W. F., Examiner

1/3 DTU-stip, 2/3 FUR/andet
01/10/2004 → 31/03/2008
Award relations: Materialedesign ved brug af tæthedsfunktionalteori og genetiske søgemetoder
Project: PhD

**Defektdynamik på atomar skala**
Vegge, T., PhD Student, Department of Energy Conversion and Storage
Jacobsen, K. W., Main Supervisor, Department of Physics
Nørskov, J. K., Examiner, Department of Physics
Gumbsch, P., Examiner
Wahnström, G., Examiner
Risø (Løn)
01/09/1998 → 03/12/2001
Award relations: Defektdynamik på atomar skala
Project: PhD
**Teoretisk modellering af nanotribologiske fænomener**
Bahn, S. R., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Schiøtz, J., Examiner, Department of Physics
Puska, M. J., Examiner
Ruitenbeek, J. V., Examiner
DTU-lønnet stipendie
01/02/1998 → 03/12/2001
Award relations: Teoretisk modellering af nanotribologiske fænomener
Project: PhD

**Undersøgelser af nye reaktionsveje for ammoniak-synteser på modificerede metal-eenkrystaller**
Dahl, S., PhD Student, Department of Physics
Chorkendorff, I., Main Supervisor, Department of Physics
Jacobsen, K. W., Examiner, Department of Physics
Grundforskningsfonden
01/08/1996 → 16/02/2000
Award relations: Undersøgelser af nye reaktionsveje for ammoniak-synteser på modificerede metal-eenkrystaller
Project: PhD

**Dissociation af N2 på Fe (III)**
Mortensen, J. J., PhD Student, Department of Physics
Nørskov, J. K., Main Supervisor, Department of Physics
Jacobsen, K. W., Supervisor, Department of Physics
Chorkendorff, I., Examiner, Department of Physics
Nørskov, J. K., Examiner
DTU-Su Stipendium, Eksperiment
01/02/1995 → 28/04/1998
Award relations: Dissociation af N2 på Fe (III)
Project: PhD

**Tribologi på Atomart Niveau**
Sørensen, M. R., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Nørskov, J. K., Supervisor, Department of Physics
Bøttiger, J., Examiner, Risø National Laboratory for Sustainable Energy
Bøttiger, J., Examiner
DTU-Su Stipendium, Eksperiment
01/09/1994 → 23/10/1997
Award relations: Tribologi på Atomart Niveau
Project: PhD

**Studier af simple molekylers klæbningskoefficient og dynamik på metal-enkrystaloverflader ved hjælp af supersoniske molekylstråler.**
Holmblad, P. M., PhD Student, Department of Physics
Chorkendorff, I., Main Supervisor, Department of Physics
Alstrup, I. A., Examiner
Jacobsen, K. W., Examiner, Department of Physics
Anden Forskningsrådsfinans.-SU
01/09/1993 → 07/06/1996
Award relations: Studier af simple molekylers klæbningskoefficient og dynamik på metal-enkrystaloverflader ved hjælp af supersoniske molekylstråler.
Project: PhD

**Energetik og dynamik af molekyler på overflader**
Jacobsen, J., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Nørskov, J. K., Supervisor, Department of Physics
Moskilde, E., Examiner, Department of Physics
DTU-Su Stipendium, Eksperiment
01/03/1993 → 29/04/1996
Award relations: Energetik og dynamik af molekyler på overflader
Project: PhD
Materialfysik på paralleldatamater
Stokbro, K., PhD Student, Department of Micro- and Nanotechnology
Jacobsen, K. W., Main Supervisor, Department of Physics
Nørskov, J. K., Supervisor, Department of Physics
Hedegård, P., Examiner
Forskningsrådsstipendium
01/08/1991 → 24/03/1995
Award relations: Materialfysik på paralleldatamater
Project: PhD

Atomic-scale modelling of interfaces in electronic devices
Jelver, L., PhD Student, Theoretical Atomic-scale Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Stokbro, K., Supervisor, Department of Micro- and Nanotechnology
Stradi, D., Supervisor, Department of Micro- and Nanotechnology
Thygesen, K. S., Supervisor, Department of Physics
Industrial PhD
01/06/2016 → 03/02/2021
Award relations: Atomic-scale modelling of interfaces in electronic devices
Project: PhD

Atomic-scale modelling of carrier dynamics in photo-excited semi-conductors
Haastrup, S., PhD Student, Department of Physics
Thygesen, K. S., Main Supervisor, Department of Physics
Jacobsen, K. W., Supervisor, Department of Physics
Schütz, J., Examiner, Department of Physics
Heine, T., Examiner
Hennig, R. G., Examiner
Institut stipendie (DTU)
01/10/2015 → 30/09/2018
Award relations: Atomic-scale modelling of carrier dynamics in photo-excited semi-conductors
Project: PhD

Computer Simulation of the 3D structure of Materials
Zhang, J., PhD Student, Department of Physics
Poulsen, H. F., Main Supervisor, Department of Physics
Voorhees, P., Supervisor
Jacobsen, K. W., Examiner, Department of Physics
Moelans, N., Examiner
Rollett, A. D., Examiner
Rollett, A. D., Examiner
Institut stipendie (DTU)
01/02/2015 → 11/04/2018
Award relations: Computer Simulation of the 3D structure of Materials
Project: PhD

Computational screening of new inorganic materials for high-efficiency solar cells
Kuhar, K., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Thygesen, K. S., Supervisor, Department of Physics
Schütz, J., Examiner, Department of Physics
Hautier, G., Examiner
Jonsson, H., Examiner
Institut stipendie (DTU)
01/11/2014 → 17/01/2018
Award relations: Computational screening of new inorganic materials for high-efficiency solar cells
Project: PhD

Modelling the environmental dependent structure of catalyst nanoparticles
Madsen, J., PhD Student, Department of Physics
Density functional theory studies of hydrodesulfurization
Šaric, M., PhD Student, Department of Physics
Jacobson, K. W., Main Supervisor, Department of Physics
Moses, P. G., Supervisor, Department of Physics
Rossmeisl, J., Supervisor, Department of Physics
Stephens, I., Examiner, Department of Physics
Lopez, N., Examiner, Department of Physics
Behrens, M., Examiner
Forskningsrådsfinansiering
01/01/2014 → 22/02/2017
Award relations: Density functional theory studies of hydrodesulfurization
Project: PhD

Transition metal sulfides as catalysis
Bengaard, H. S., PhD Student, Department of Physics
Nørskov, J. K., Main Supervisor, Department of Physics
Rostrup-Nielsen, J., Supervisor, Risø National Laboratory for Sustainable Energy
Jacobson, K. W., Examiner, Department of Physics
Lundqvist, B. I., Examiner
Schlögl, R., Examiner
Rostrup-Nielsen, J., Supervisor
Forskerakademiets Samfinansier
01/02/1998 → 02/04/2002
Award relations: Transition metal sulfides as catalysis
Project: PhD

Dislokationers struktur og dynamik
Rasmussen, T., PhD Student, Department of Physics
Jacobson, K. W., Main Supervisor, Department of Physics
Skriver, H. L., Examiner, Department of Physics
Risø (Løn)
01/01/1995 → 25/02/1998
Award relations: Dislokationers struktur og dynamik
Project: PhD

Design of Novel Materials for Energy Storage
Voss, J., PhD Student, Department of Physics
Nørskov, J. K., Main Supervisor, Department of Physics
Vegge, T., Supervisor, Department of Physics
Jacobson, K. W., Examiner, Department of Physics
Jonsson, H., Examiner
Manninen, M. J., Examiner
Risø (Løn)
01/08/2005 → 02/02/2009
Award relations: Design of Novel Materials for Energy Storage
Project: PhD

Struktur og mekaniske egenskaber af nanokrystallinske materialer
Christiansen, J., PhD Student, Department of Physics
Schiøtz, J., Main Supervisor, Department of Physics
Jacobson, K. W., Supervisor, Department of Physics
Leffers, T., Supervisor, Risø National Laboratory for Sustainable Energy
Nørskov, J. K., Examiner, Department of Physics
Bøttiger, J., Examiner, Risø National Laboratory for Sustainable Energy
Devincere, B., Examiner
Leffers, T., Supervisor
Bøttiger, J., Examiner
Risø (Løn)
01/04/2000 → 01/12/2003
Award relations: Struktur og mekaniske egenskaber af nanokrystallinske materialer
Project: PhD

Materials Informatics
Landis, D. D., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Bligaard, T., Supervisor, Department of Physics
Schiøtz, J., Examiner, Department of Physics
Enkovaara, J., Examiner
Moses, P. G., Examiner, Department of Physics
Offentlig finansiering
01/06/2008 → 30/04/2012
Award relations: Materials Informatics
Project: PhD

Electronic Properties of Transition Metal Dichalcogenide Heterostructures
Latini, S., PhD Student, Department of Physics
Thygesen, K. S., Main Supervisor, Department of Physics
Jacobsen, K. W., Examiner, Department of Physics
Gatti, M., Examiner
Wehling, T. O., Examiner
Grundforskningsfonden
15/09/2013 → 12/12/2016
Award relations: Electronic Properties of Transition Metal Dichalcogenide Heterostructures
Project: PhD

Metan aktivering
Abild-Pedersen, F., PhD Student, Department of Physics
Nørskov, J. K., Main Supervisor, Department of Physics
Jacobsen, K. W., Examiner, Department of Physics
Lundqvist, B. I., Examiner
Grundforskningsfonden
01/02/2002 → 28/09/2005
Award relations: Metan aktivering
Project: PhD

Dislokationkernels struktur og dynamik
Frederiksen, S. L., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Schiøtz, J., Supervisor, Department of Physics
Nørskov, J. K., Examiner, Department of Physics
Finnis, M. W., Examiner
Leffers, T., Examiner, Risø National Laboratory for Sustainable Energy
Leffers, T., Examiner
Grundforskningsfonden
01/08/2000 → 26/02/2004
Award relations: Dislokationkernels struktur og dynamik
Project: PhD

DFT-Simulations of low temperature fuel cells catalysis
Hansen, M. H., PhD Student, Department of Physics
Thygesen, K. S., Main Supervisor, Department of Physics
Rossmeisl, J., Supervisor, Department of Physics
Jacobsen, K. W., Examiner, Department of Physics
Gross, A., Examiner
Koper, M. T. M., Examiner
Forskningsrådsfinansiering
15/05/2013 → 25/08/2016
Award relations: DFT-Simulations of low temperature fuel cells catalysis
Project: PhD

Modeling of level alignment and charge separation at donor/acceptor interfaces
Ømose, K. B., PhD Student, Department of Physics
Thygesen, K. S., Main Supervisor, Department of Physics
Jacobsen, K. W., Supervisor, Department of Physics
Vegge, T., Examiner, Department of Physics
Boschloo, G. K., Examiner
Troisi, A., Examiner
Forskningsrådsfinansiering
01/08/2012 → 23/10/2015
Award relations: Modeling of level alignment and charge separation at donor/acceptor interfaces
Project: PhD

Microfluidics of Sugar Transport in Trees and in Biomimetic Devices
Rademaker, H., PhD Student, Department of Physics
Bohr, T., Main Supervisor, Department of Physics
Jensen, K. H., Supervisor, Department of Physics
Jacobsen, K. W., Examiner, Department of Physics
Clanet, C., Examiner
Holbrook, N. M., Examiner
Samfinansieret - Andet
15/09/2013 → 26/10/2016
Award relations: Microfluidics of Sugar Transport in Trees and in Biomimetic Devices
Project: PhD

Molecular Dynamics simulations in materials science
Schätz, J., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Nørskov, J. K., Supervisor, Department of Physics
Finnis, M. W., Examiner
Hedegård, P., Examiner
DTU-stipendium
01/02/1992 → 22/05/1995
Award relations: Molecular Dynamics simulations in materials science
Project: PhD

Teori for STM
Brandbyge, M., PhD Student, Center for Nanostructured Graphene
Jacobsen, K. W., Main Supervisor, Department of Physics
Svane, A., Examiner
Grundforskningsfonden-SU
01/03/1994 → 26/08/1997
Award relations: Teori for STM
Project: PhD

Density Functional Calculations and Molecular Modeling of Biological Ammonia Synthesis
Rod, T. H., PhD Student, Department of Physics
Nørskov, J. K., Main Supervisor, Department of Physics
Jacobsen, K. W., Examiner, Department of Physics
Stoltze, P., Examiner, Department of Physics
Grundforskningsfonden-SU
01/12/1996 → 24/03/2000
Award relations: Density Functional Calculations and Molecular Modeling of Biological Ammonia Synthesis
Project: PhD
**Teori for Quantum Devices**

Johnsen, K., PhD Student, Department of Micro- and Nanotechnology
Jauho, A., Main Supervisor, Department of Micro- and Nanotechnology
Jacobsen, K. W., Examiner
Smith, H., Examiner

Mic-Finansieret-SU
01/09/1995 → 10/08/1999
Award relations: Teori for Quantum Devices
Project: PhD

**Theory of electrokinetic power generation in portable nanofluidic devices**

Andersen, M. B., PhD Student, Department of Micro- and Nanotechnology
Bruus, H., Main Supervisor, Department of Micro- and Nanotechnology
Jacobsen, K. W., Examiner
Eijkel, J. C. T., Examiner
Yariv, E., Examiner

1/3 DTU-stip, 2/3 FUR/andet
01/04/2009 → 19/06/2012
Award relations: Theory of electrokinetic power generation in portable nanofluidic devices
Project: PhD

**Interatomare vekselvirkninger i metaller.**

Christensen, A., PhD Student, National Institute of Aquatic Resources
Nørskov, J. K., Main Supervisor, Department of Physics
Jacobsen, K. W., Supervisor, Department of Physics

DTU-Su Stipendium, Eksperiment
01/09/1993 → 27/01/1997
Award relations: Interatomare vekselvirkninger i metaller.
Project: PhD

**Density functional theory used on biological systems**

Rossmeisl, J., PhD Student, Center for Atomic-scale Materials Design
Nørskov, J. K., Main Supervisor, Department of Physics
Jacobsen, K. W., Supervisor, Department of Physics
Skriver, H. L., Examiner, Department of Physics
Pettersson, L. G. M., Examiner
Scheffler, M., Examiner

DTU-lønnet stipendie
01/02/2000 → 12/02/2004
Award relations: Density functional theory used on biological systems
Project: PhD

**Theoretical study of ammonia synthesis under ambient conditions**

Petzold, V. G., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Bligaard, T., Supervisor, Department of Physics
Nørskov, J. K., Supervisor, Department of Physics
Thygesen, K. S., Examiner, Department of Physics
Hyldgaard, P., Examiner
Reuter, K., Examiner

DTU-lønnet stipendie
01/04/2007 → 02/03/2011
Award relations: Theoretical study of ammonia synthesis under ambient conditions
Project: PhD

**Elektrontransport i Nanostrukturen**

Rostgaard, C., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Thygesen, K. S., Supervisor, Department of Physics
Bligaard, T., Examiner, Department of Physics
Gao, S., Examiner
van Leeuwen, R., Examiner
DTU-lønnet stipendie
15/08/2006 → 10/02/2010
Award relations: Elektrontransport i Nanostrukturer
Project: PhD

Nanostrukturers opbygning, dynamik og transportegenskaber
Thygesen, K. S., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Nørskov, J. K., Examiner, Department of Physics
Gonze, X., Examiner
Stokbro, K., Examiner, Department of Micro- and Nanotechnology

DTU-lønnet stipendie
01/02/2002 → 06/06/2005
Award relations: Nanostrukturers opbygning, dynamik og transportegenskaber
Project: PhD

Quantum description of enzyme function
Hinnemann, B., PhD Student, Department of Physics
Nørskov, J. K., Main Supervisor, Department of Physics
Jacobsen, K. W., Supervisor, Department of Physics
Schietz, J., Examiner, Department of Physics
Stoltze, P., Examiner, Department of Physics
Trout, B. L., Examiner

DTU-lønnet stipendie
01/01/2001 → 23/03/2004
Award relations: Quantum description of enzyme function
Project: PhD

Struktur og elektriske egenskaber af molekyler ved overflader
Bollinger, M., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Schietz, J., Examiner, Department of Physics
Hylland, P., Examiner
Nieminen, R., Examiner

DTU-lønnet stipendie
01/09/1999 → 15/11/2002
Award relations: Struktur og elektriske egenskaber af molekyler ved overflader
Project: PhD

Vekselvirkningseffekter i lavdimensionale elektronsystemer
Mortensen, N. A., PhD Student, Department of Micro- and Nanotechnology
Jauho, A., Main Supervisor, Department of Micro- and Nanotechnology
Flensberg, K., Supervisor
Jacobsen, K. W., Examiner
Büttiker, M., Examiner
Jonson, M. S., Examiner

DTU-lønnet stipendie
01/01/1999 → 25/09/2001
Award relations: Vekselvirkningseffekter i lavdimensionale elektronsystemer
Project: PhD

Modelling the Shape and Reactivity of Metallic Nanoparticles
Gavnholt, J., PhD Student, Department of Physics
Schietz, J., Main Supervisor, Department of Physics
Jacobsen, K. W., Examiner, Department of Physics
Hylland, P., Examiner
Häkkinen, H., Examiner

DTU-lønnet stipendie
01/02/2006 → 05/05/2009
Award relations: Modelling the Shape and Reactivity of Metallic Nanoparticles
Project: PhD
Alternative Routes to Ammonia Synthesis
Skulason, E., PhD Student, Department of Physics
Nørskov, J. K., Main Supervisor, Department of Physics
Bligaard, T., Supervisor, Department of Physics
Jonsson, H., Supervisor, Department of Physics
Jacobsen, K. W., Examiner, Department of Physics
Gross, A., Examiner
Forskningsrådsfinansiering
01/09/2005 → 28/10/2009
Award relations: Alternative Routes to Ammonia Synthesis
Project: PhD

Inclusion of dispersion effects in density functional theory: Development and application
Møgelhøj, A., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Nørskov, J. K., Supervisor, Department of Physics
Brandbyge, M., Examiner, Department of Micro- and Nanotechnology
Jonsson, H., Examiner
Mikkelsen, K. V., Examiner
Institut stipendie (DTU)
01/07/2009 → 22/08/2012
Award relations: Inclusion of dispersion effects in density functional theory: Development and application
Project: PhD

Katalytiske og elektroniske egenskaber af metalnanopartikler
Larsen, A. H., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Thygesen, K. S., Supervisor, Department of Physics
Rossmieisl, J., Examiner, Department of Physics
Grönbeck, H., Examiner
Manninen, M. J., Examiner
Institut stipendie (DTU) Samf.
01/09/2008 → 20/01/2012
Award relations: Katalytiske og elektroniske egenskaber af metalnanopartikler
Project: PhD

Accurate treatment of nanoelectronics through improved description of van der Waals Interactions
Kelkkanen, K. A., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Lundqvist, B. I., Supervisor
Nørskov, J. K., Supervisor, Department of Physics
Rossmieisl, J., Examiner, Department of Physics
Mahan, G. D., Examiner
Michaëlides, A., Examiner
Eksternt finansieret virksomhed
01/02/2008 → 20/04/2011
Award relations: Accurate treatment of nanoelectronics through improved description of van der Waals Interactions
Project: PhD

Computational Screening of Energy Materials
Pandey, M., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Thygesen, K. S., Supervisor, Department of Physics
Schiøtz, J., Examiner, Department of Physics
Jonsson, H., Examiner
Wahnström, G., Examiner
1/3 FUU, 1/3 inst 1/3 Andet
01/08/2012 → 30/09/2015
Award relations: Computational Screening of Energy Materials
Project: PhD
Computational search for new light harvesting materials for solar-to-fuel energy conversion
Castelli, I. E., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Thygesen, K. S., Supervisor, Department of Physics
Schietz, J., Examiner, Department of Physics
Marzari, N., Examiner
Pedersen, T. G., Examiner, Risø National Laboratory for Sustainable Energy
Pedersen, T. G., Examiner
Forskningsrådsfinansiering
01/06/2010 → 26/09/2013
Award relations: Computational search for new light harvesting materials for solar-to-fuel energy conversion
Project: PhD

Design of zeolite catalysts for selective benzene to cyclohexene hydrogenation
Wellendorff, J. B., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Bligaard, T., Supervisor, Department of Physics
Rossmeisl, J., Examiner, Department of Physics
Hellman, A., Examiner
Michaelides, A., Examiner
Institut, samfinansiering
01/08/2009 → 21/09/2012
Award relations: Design of zeolite catalysts for selective benzene to cyclohexene hydrogenation
Project: PhD

Electronic transport and atomic dynamics in graphene-based nanostructures - theory and simulation
Christensen, R. B., PhD Student, Department of Micro- and Nanotechnology
Brandbyge, M., Main Supervisor, Department of Micro- and Nanotechnology
Jacobsen, K. W., Examiner
Paulsson, M., Examiner
Solomon, G., Examiner
Forskningsrådsfinansiering
15/08/2011 → 07/05/2015
Award relations: Electronic transport and atomic dynamics in graphene-based nanostructures - theory and simulation
Project: PhD

Interfacial Electron Transfer of Large Transition Metal Complexes in Condensed Matter Environments
Jönsson, E. O., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Thygesen, K. S., Supervisor, Department of Physics
Ulstrup, J., Supervisor
Rossmeisl, J., Examiner, Department of Physics
Jonsson, H., Examiner
Sprik, M., Examiner
Institut stipendie (DTU)
01/10/2010 → 25/04/2014
Award relations: Interfacial Electron Transfer of Large Transition Metal Complexes in Condensed Matter Environments
Project: PhD

Water Splitting Reaction at Semiconductor Surfaces
Zawadzki, P., PhD Student, Department of Physics
Nørskov, J. K., Main Supervisor, Department of Physics
Jacobsen, K. W., Supervisor, Department of Physics
Rossmeisl, J., Supervisor, Department of Physics
Chorkendorff, I., Examiner, Department of Physics
Jonsson, H., Examiner
Marzari, N., Examiner
Forskningsrådsfinansiering
01/01/2009 → 23/02/2012
Award relations: Water Splitting Reaction at Semiconductor Surfaces
Project: PhD
Computational modelling of electron transport at metal-organic interfaces
Jin, C., PhD Student, Department of Physics
Thygesen, K. S., Main Supervisor, Department of Physics
Jacobsen, K. W., Examiner, Department of Physics
Pauly, F., Examiner
Ratner, M. A., Examiner
Forskningsrådsfinansiering
15/02/2012 → 21/09/2015
Award relations: Computational modelling of electron transport at metal-organic interfaces
Project: PhD

Plastic Deformation of Metallic Glasses
Paduraru, A., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Schiøtz, J., Supervisor, Department of Physics
Nørskov, J. K., Examiner, Department of Physics
Evangelakis, G., Examiner
Wahnström, G., Examiner
1/3 DTU-stip, 2/3 FUR/andet
01/02/2005 → 31/03/2008
Award relations: Plastic Deformation of Metallic Glasses
Project: PhD

Theoretical Investigation of Plasmonic Materials using Electronic Structure Methods
Winther, K. T., PhD Student, Department of Physics
Thygesen, K. S., Main Supervisor, Department of Physics
Jacobsen, K. W., Supervisor, Department of Physics
Schiøtz, J., Examiner, Department of Physics
García de Abajo, F. J., Examiner
Puska, M. J., Examiner
Institut stipendie (DTU)
01/09/2011 → 13/08/2015
Award relations: Theoretical Investigation of Plasmonic Materials using Electronic Structure Methods
Project: PhD

Development and testing of new exchange-correlation functionals
Lundgård, K. T., PhD Student, Department of Physics
Jacobsen, K. W., Main Supervisor, Department of Physics
Thygesen, K. S., Supervisor, Department of Physics
Schiøtz, J., Examiner, Department of Physics
Moses, P. G., Examiner, Department of Physics
Tkatchenko, A., Examiner
Institut stipendie (DTU)
01/02/2011 → 20/03/2014
Award relations: Development and testing of new exchange-correlation functionals
Project: PhD

Electron Transport and Chemistry of Graphene
Vanin, M., PhD Student, Department of Physics
Thygesen, K. S., Main Supervisor, Department of Physics
Jacobsen, K. W., Supervisor, Department of Physics
Brandbyge, M., Examiner, Department of Physics
Brockes, G. H. L. A., Examiner
Hornekær, L., Examiner
Institut stipendie (DTU)
01/09/2008 → 30/09/2011
Award relations: Electron Transport and Chemistry of Graphene
Project: PhD
**Design of functional nanomaterials**

To establish a research collaboration encompassing all steps in the development of new functional nanomaterials: design, synthesis, characterization, and testing. The common aim of the proposal is the development of rational design strategies for nano-structured materials.

Nørskov, J. K., Project Manager, Department of Physics  
Jacobsen, K. W., Project Participant, Department of Physics  
Chorkendorff, I., Project Participant, Department of Physics  
Nielsen, J. H., Project Participant, Department of Physics  
Horch, S., Project Participant, Department of Physics  
Schiatz, J., Project Participant, Department of Physics  
Quaade, U., Project Participant, Department of Physics  
Christensen, C. H., Project Participant, Department of Chemistry  
Ulstrup, J., Project Participant, Department of Chemistry  
Johannessen, T., Project Participant, Department of Chemical and Biochemical Engineering, Administration  
Bøggild, P., Project Participant, Department of Micro- and Nanotechnology  
Pedersen, A. S., Project Participant, Risø National Laboratory for Sustainable Energy  
Linderoth, S., Project Participant, Risø National Laboratory for Sustainable Energy  
Mogensen, M., Project Participant, Risø National Laboratory for Sustainable Energy  
Vegge, T., Project Participant, Risø National Laboratory for Sustainable Energy  
Pryds, N., Project Participant, Risø National Laboratory for Sustainable Energy  
Henriksen, P. V., Project Participant  
Kuhn, L. T., Project Participant, Risø National Laboratory for Sustainable Energy  

**Project ID:** 20195  
**Forskningsrådene - Andre:** DKK9,290,000.00  
**01/01/2005 → 31/12/2008**  
**Award relations:** Design of functional nanomaterials  
**Project:** Research

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**Mechanical properties of materials**

The aim of the project is to understand the mechanical properties of materials, in particular metals and alloys, by studying the atomic structure using computer simulations. The simulations are mostly based on the effective medium theory. The study focusses on crystal defects (in particular dislocations, cracks, grain boundaries and surfaces) and their mutual interactions. It includes both studies of idealized geometries such as a single crack near a grain boundary, and more realistic geometries such as nanocrystalline metals.

Schiatz, J., Project Manager, Department of Physics  
Jacobsen, K. W., Project Participant, Department of Physics  
Vegge, T., Project Participant, Department of Physics  
Leffers, T., Project Participant, Risø National Laboratory for Sustainable Energy  
Pedersen, O. B., Project Participant, Risø National Laboratory for Sustainable Energy  
Bilde-Sørensen, J., Project Participant, Risø National Laboratory for Sustainable Energy  

**Project ID:** 20195  
**Award relations:** Design of functional nanomaterials  
**Project:** Mechanical properties of materials

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**Electronic structure and reactivity**

The project aims at developing models of adsorption and reaction at surfaces. The basis is detailed self-consistent calculations using density functional theory with a non-local desorption of exchange and correlation. Models based on the effective medium theory and the Newns-Andersen model are developed to identify the important parameters determining the reactivity of a given system. The theoretical work is closely coupled to experiments on model systems and in industry. The systems studied include clean metals, alloys, transition metal sulfides, and models of enzymes.

Nørskov, J. K., Project Manager, Department of Physics  
Jacobsen, K. W., Project Participant, Department of Physics  
Stoltze, P., Project Participant, Department of Physics  
Byskov, L. S., Project Participant, Department of Physics  
Rod, T. H., Project Participant, Department of Physics  
Mavrikakis, M., Project Participant, Department of Physics  
Bengaard, H. S., Project Participant, Department of Physics  
Logadóttir, Á., Project Participant, Department of Physics  
Bollinger, M., Project Participant, Department of Physics  
Besenbacher, F., Project Participant, Aarhus University  
Stensgaard, I., Project Participant, Aarhus University  
Laegsgaard, E., Project Participant, Aarhus University  
Clausen, B. S., Project Participant, Haldor Topsoe AS  
Pirovano, V., Project Participant  

**Award relations:** Design of functional nanomaterials  
**Project:** Electronic structure and reactivity

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Metallic nanostructures
The aim of the project is to study the mechanisms behind the formation of metallic nanostructures and to investigate the structural, mechanical, and electrical properties of nanostructures. The project has involved studies of atomic mobility at surfaces and the aggregation of adatoms into islands of various morphologies. Also investigations of mechanical and electrical aspects of a scanning-tunneling-microscope tip interacting with a metal surface have been carried out. In particular the tip-surface system has been used as a model system for nanotribological considerations. Finally, a series of simulations of plastic deformation of nanophase metals have been performed.

Stoltze, P., Project Manager, Department of Physics
Jacobsen, K. W., Project Participant, Department of Physics
Nørskov, J. K., Project Participant, Department of Physics
Schiøtz, J., Project Participant, Department of Physics
Nielsen, O. H., Project Participant, Department of Physics
Vegge, T., Project Participant, Department of Physics
Bahn, S. R., Project Participant, Department of Physics
Lorensen, H. Q., Project Participant, Department of Physics
Bollinger, M., Project Participant, Department of Physics
Besenbacher, F., Project Participant, Aarhus University
Stensgaard, I., Project Participant, Aarhus University
Laegsgaard, E., Project Participant, Aarhus University

Simulations of alloy dynamics and kinetics
In this project the macroscopic properties of systems are determined based on description at the atomic level through large-scale computer simulations. The main topics of interest are the stability, structure and dynamics of alloys and of metal surfaces and the relation between observed kinetics and reaction mechanism for industrial catalytic reactions. Some of the software for simulation and visualization is available at http://www.fysik.dtu.dk/camp-sd.html

Stoltze, P., Project Manager, Department of Physics
Jacobsen, K. W., Project Participant, Department of Physics
Nørskov, J. K., Project Participant, Department of Physics
Chorkendorff, I., Project Participant, Department of Physics
Schiøtz, J., Project Participant, Department of Physics
Christoffersen, E., Project Participant, Department of Physics
Dahl, S., Project Participant, Department of Physics
Clausen, B., Project Participant, Haldor Topsoe AS
Jacobsen, C., Project Participant, Haldor Topsoe AS
Sehested, J., Project Participant, Haldor Topsoe AS

Computational Atomic-scale Materials Physics
Installation and operation of a Linux cluster

Jacobsen, K. W., Project Manager, Department of Physics
Ductile BMG Composites

Bulk metallic glasses are an exciting new class of materials with high yield stress and low elastic moduli, making them interesting in situations where mechanical energy is stored (springs etc). Unfortunately, they are quite brittle, and fail through the formation of shear bands. We use molecular dynamics simulations to study the deformation mechanisms and shear band formation with the goal of designing less brittle metallic glasses.

Jacobsen, K. W., Project Manager, Department of Physics
Schiøtz, J., Project Participant, Department of Physics
Yavari, R., Contact Person, Centre National de Recherche Scientifique (CNRS), Institut National Polytechnique de Grenoble (INPG),

Center for Atomic-scale Materials Physics (CAMP)

The general theme for the research in CAMP is the study of metallic nano-structures and their properties by a closely coupled experimental and theoretical approach. In the present report the research is organized under three main headings: 1. Nano-structures, focused on an understanding of structural, mechanical, and electrical properties of nano-structures. 2. Surface alloys and surface chemical properties, focused on the understanding, design, and synthesis of surfaces and the possibility of modifying and controlling their chemical reactivity. 3. Biomolecules, focused on the understanding of the structure and interactions within proteins, their enzymatic function, and their interactions with solid surfaces.

Nørskov, J. K., Project Manager
Jacobsen, K. W., Project Participant, Department of Physics
Skriver, H. L., Project Participant, Department of Physics
Chorkendorff, I., Project Participant, Department of Physics
Schiøtz, J., Project Participant, Department of Physics
Horch, S., Project Participant, Department of Physics
Nielsen, J. H., Project Participant, Department of Physics
Quaade, U., Project Participant, Department of Physics
Besenbacher, F., Project Participant, Aarhus University
Stensgaard, I., Project Participant, Aarhus University
Laegsgaard, E., Project Participant, Aarhus University
Hammer, B., Project Participant, Aarhus University

Danish Center for Scientific Computing (DCSC) - 2

Installation and operation of a Linux cluster. The machine is dedicated to ambitious research projects within material physics, heterogeneous catalysis and electrochemistry.

Jacobsen, K. W., Project Manager, Department of Physics

Project ID: 20172
Forsk. Private danske - Andre: DKK4,000,000.00
01/01/2004 → 31/12/2007
Award relations: Danish Center for Scientific Computing (DCSC) - 2
Project: Research