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Publications:

Computational materials design from first principles

General information
State: Published
Organisations: Department of Physics, Department of Chemistry, Center for Nanoteknologi
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Scopus rating (2008): SJR 2.201 SNIP 2.076
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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BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.021 SNIP 2.177
Atomic and magnetic configurational energetics by the generalized perturbation method

It is shown that, using the generalized perturbation method (GPM) with screened Coulomb interactions that ensures its consistency with the force theorem, one is able to obtain effective interactions that yield an accurate and physically transparent description of configurational energetics in the framework of the Korringa-Kohn-Rostoker method within the atomic sphere and coherent potential approximations. This is demonstrated with calculations of ordering energies, short-range order parameters, and transition temperatures in the CuZn, CuAu, CuPd, and PtCo systems. Furthermore, we show that the GPM can be used to obtain Heisenberg exchange interaction parameters, which, for instance, capture very well the magnetic configurational energy in bcc Fe.

General information

State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Linköping University, Uppsala University
Authors: Ruban, A. V. (Intern), Shallcross, S. (Ekstern), Simak, S. (Ekstern), Skriver, H. L. (Intern)
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Main Research Area: Technical/natural sciences

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Scopus rating (2013): SJR 2.785 SNIP 1.339
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.206 SNIP 1.394
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.382 SNIP 1.438
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 3.417 SNIP 1.451
BFI (2009): BFI-level 2
Local lattice relaxations in random metallic alloys: Effective tetrahedron model and supercell approach

We present a simple effective tetrahedron model for local lattice relaxation effects in random metallic alloys on simple primitive lattices. A comparison with direct ab initio calculations for supercells representing random Ni_{0.5}Pt_{0.5} and Cu_{0.25}Au_{0.75} alloys as well as the dilute limit of Au-rich CuAu alloys shows that the model yields a quantitatively accurate description of the relaxation energies in these systems. Finally, we discuss the bond length distribution in random alloys.
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.

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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.
Screened Coulomb interactions in metallic alloys. II. Screening beyond the single-site and atomic-sphere approximations

A quantitative description of the configurational part of the total energy of metallic alloys with substantial atomic size difference cannot be achieved in the atomic-sphere approximation: It needs to be corrected at least for the multipole-moment interactions in the Madelung part of the one-electron potential and energy. In the case of a random alloy such interactions can be accounted for only by lifting the atomic-sphere and single-site approximations, in order to include the polarization due to local environment effects. Nevertheless, a simple parametrization of the screened Coulomb interactions for the ordinary single-site methods, including the generalized perturbation method, is still possible. We obtained such a parametrization for bulk and surface NiPt alloys, which allows one to obtain quantitatively accurate effective interactions in this system.
Screened Coulomb interactions in metallic alloys. I. Universal screening in the atomic-sphere approximation

We have used the locally self-consistent Green's-function (LSGF) method in supercell calculations to establish the distribution of the net charges assigned to the atomic spheres of the alloy components in metallic alloys with different compositions and degrees of order. This allows us to determine the Madelung potential energy of a random alloy in the single-site, mean-field approximation. The Madelung potential makes density-functional calculations by the conventional single-site, coherent potential approximation practically identical to the more rigorous LSGF supercell results obtained with a single-site local interaction zone. We demonstrate that the basic mechanism that governs the charge distribution is the screening of the net charges of the alloy components that makes the direct Coulomb interactions short ranged. In the atomic-sphere approximation, this screening appears to be almost independent of the alloy composition, lattice spacing, and crystal structure. A formalism which allows a consistent treatment of the screened Coulomb interactions within the single-site mean-field approximation is outlined. We also derive the contribution of the screened Coulomb interactions to the S-(2) formalism and the generalized perturbation method.
Scopus rating (2008): SJR 2.982 SNIP 1.524
Scopus rating (2007): SJR 2.923 SNIP 1.546
Scopus rating (2006): SJR 2.796 SNIP 1.56
Scopus rating (2005): SJR 2.763 SNIP 1.607
Scopus rating (2004): SJR 2.742 SNIP 1.606
Scopus rating (2003): SJR 2.75 SNIP 1.536
Scopus rating (2002): SJR 2.788 SNIP 1.706
Scopus rating (2001): SJR 2.946 SNIP 1.635
Scopus rating (2000): SJR 2.986 SNIP 1.631
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ELECTRONIC-STRUCTURE, DENSITY-FUNCTIONAL THEORY, MADELUNG LATTICE, GENERALIZED PERTURBATION-THEORY, COHERENT-POTENTIAL APPROXIMATION, GROUND-STATE, RANDOM SUBSTITUTIONAL ALLOYS, EFFECTIVE CLUSTER INTERACTIONS, ORDERING ENERGIES, DISORDERED ALLOYS

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Surface Alloys and Alloy Surfaces

General information
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Organisations: Department of Physics
Authors: Ruban, A. (Intern), Skriver, H. L. (Intern), Nørskov, J. K. (Intern)
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Anode Materials for Low-Temperature Fuel Cells: A Density Functional Theory Study

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Organisations: Department of Physics
Authors: Christoffersen, E. (Intern), Liu, P. (Intern), Ruban, A. (Intern), Skriver, H. L. (Intern), Nørskov, J. K. (Intern)
Pages: 123-131
Publication date: 2001
Main Research Area: Technical/natural sciences

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BFI (2017): BFI-level 2
Application of the Exact Muffin-Tin Orbitals theory: The spherical cell approximation

General information
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Organisations: Department of Physics
Authors: Vitos, L. (Intern), Skriver, H. L. (Intern), Johansson, B. (Ekstern), Kollár, J. (Ekstern)
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Exchange energy in the local Airy gas approximation

The Airy gas model of the edge electron gas is used to construct an exchange-energy functional that is an alternative to those obtained in the local-density and generalized-gradient approximations. Test calculations for rare-gas atoms, molecules, solids, and surfaces show that the Airy gas functional performs better than the local-density approximation in all cases and better than the generalized-gradient approximation for solids and surfaces.
SEMICONDUCTORS, ACCURATE, GENERALIZED GRADIENT APPROXIMATION, CHARGE-DENSITY, SURFACES, ALL-ELECTRON, DENSITY-FUNCTIONAL-THEORY

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From ASA towards full potential

General information
State: Published
Organisations: Department of Physics
Authors: Vitos, L. (Intern), Skriver, H. L. (Intern)
Publication date: 2000

Host publication information
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Place of publication: Berlin
Publisher: Springer-Verlag
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 177080
Publication: Research - peer-review › Article in proceedings – Annual report year: 2000
Local kinetic-energy density of the Airy gas

The Airy gas model is used to derive an expression for the local kinetic energy in the linear potential approximation. The expression contains an explicit Laplacian term \(2/5(\hbar^2/2m)\nabla^2(\rho_0)\) that, according to jellium surface calculations, must be a universal feature of any accurate local description. Applied to the noble gases the expression reduces the errors by a factor of 50 over previous results obtained by the linear potential approximation.
Metal surfaces: Surface, step and kink formation energies

We review the surface, step, and kink energies in monoatomic metallic systems. A systematic comparison is given between the theoretical results based on density functional theory and available experimental data. Our calculated values are used to predict the equilibrium shapes of small metal particles, monoatomic surface islands, and the instability of different surface geometries.
Stability of fcc(110) transition and noble metal surfaces

General information
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Organisations: Department of Physics
Authors: Vitos, L. (Intern), Johansson, B. (Ekstern), Skriver, H. L. (Intern), Kollár, J. (Ekstern)
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Scopus rating (2012): SJR 1.022 SNIP 1.647
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Scopus rating (2011): SJR 0.996 SNIP 1.46
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.961 SNIP 1.257
BFI (2009): BFI-level 2
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Scopus rating (2004): SJR 0.915 SNIP 1.06
Scopus rating (2003): SJR 0.61 SNIP 0.775
Scopus rating (2002): SJR 0.576 SNIP 0.705
Scopus rating (2001): SJR 0.539 SNIP 0.752
Scopus rating (2000): SJR 0.489 SNIP 0.761
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Original language: English
Source: orbit
Source-ID: 177074
Steps, kinks, and segregation at metallic surfaces

General information
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Organisations: Department of Physics
Authors: Skriver, H. L. (Intern), Ruban, A. (Intern), Nørskov, J. K. (Intern), Vitos, L. (Intern), Kollár, J. (Ekstern)
Pages: 193
Publication date: 2000
Main Research Area: Technical/natural sciences

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Calculated surface segregation in transition metal alloys

General information
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Organisations: Department of Physics
Authors: Ruban, A. (Intern), Skriver, H. L. (Intern)
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BFI (2008): BFI-level 2
Scopus rating (2008): SJR 0.919 SNIP 1.3
Scopus rating (2007): SJR 0.682 SNIP 1.029
Scopus rating (2006): SJR 0.852 SNIP 1.474
First-principles calculations of the vacancy formation energy in transition and noble metals

Abstract: The vacancy formation energy and the vacancy formation volume of the 3d, 4d, and 5d transition and noble metals have been calculated within the local-density approximation. The calculations employ the order-N locally self-consistent Green's-function method in conjunction with a supercell approach and include electrostatic multipole corrections to the atomic sphere approximation. The results are in excellent agreement with available full-potential calculations and with the vacancy formation energies obtained in positron annihilation measurements. The variation of the vacancy formation energy through a transition-metal series and the effects of crystal and magnetic structure are investigated and discussed. [S0163-1829(99)07717-6].

General information

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Organisations: Department of Physics, Theoretical Atomic-scale Physics, Uppsala University
Authors: Korzhavyi, P. (Ekstern), Abrikosov, I. A. (Ekstern), Johansson, B. (Ekstern), Ruban, A. (Intern), Skriver, H. L. (Intern)
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Bibliographical note
Interface magnetism of 3d transition metals
The layered resolved magnetic spin moments of the magnetic 3d bilayer interfaces Fe/V bcc, Fe/Co bcc, Fe/Cu bcc, Co/V bcc, Co/Ni fcc, Ni/Cr fcc, Ni/Cu fcc, and the magnetic surfaces Fe bcc, Co bcc, Co fee, and Ni fee are calculated for the (001), (011), and (111) orientations by means of a first-principles Green's function method. It is shown how the magnetic profiles around the bilayer interfaces and surfaces directly can be used to predict the magnetization of more complex systems such as magnetic multilayers and clusters. Furthermore, it is shown how the magnetic interface moments can be estimated from data of the corresponding binary bulk alloys. The behavior of interface magnetism can thus be traced back to the understanding of magnetism in bulk alloys. [S0163-1829(99)04005-9].

Magnetic interlayer coupling and interaction between interface states in a quantum-well system

Magnetic interlayer coupling and interaction between interface states in a quantum-well system
Surface segregation energies in transition-metal alloys

We present a database of 24 x 24 surface segregation energies of single transition metal impurities in transition-metal hosts obtained by a Green's-function linear-muffin-tin-orbitals method in conjunction with the coherent potential and atomic sphere approximations including a multipole correction to the electrostatic potential and energy. We use the database to establish the major factors which govern surface segregation in transition metal alloys. We find that the calculated trends are well described by Friedel's rectangular state density model and that the few but significant deviations from the simple trends are caused by crystal structure effects. [S0163-1829(99)05424-7].
The formation energy for steps and kinks on cubic transition metal surfaces
We have used our first-principles database of surface energies for metals in conjunction with the concept of vicinal surfaces to derive the energies of formation of monoatomic steps and corresponding kinks on close-packed surface facets of bcc and fcc transition metals. The entries in the database allow for a direct calculation of the energies of a number of important steps. For the remaining steps and for all the kinks the energies of formation have been estimated from pair potential expansions of the entries in the database. (C) 1999 Elsevier Science B.V. All rights reserved.
Co-segregation at the surface of Pb-Bi-Ni alloys: combined ab initio) and Monte Carlo study

Crystal-Structure Contribution to the Solid Solubility in Transition Metal Alloys

The solution energies of 4d metals in other 4d metals as well as the bcc-hcp structural energy differences in random 4d alloys are calculated by density functional theory. It is shown that the crystal structure of the host plays a crucial role in the solid solubility. A local virtual bond approximation accounts for the calculated solution energies and explains the
substantial reduction in structural energy caused by randomness.
Kinetic-energy functionals studied by surface calculations

The self-consistent jellium model of metal surfaces is used to study the accuracy of a number of semilocal kinetic-energy functionals for independent particles. It is shown that the poor accuracy exhibited by the gradient expansion approximation and most of the semiempirical functionals in the low density, high gradient limit may be substantially improved by including locally a von Weizsacker term. Based on this, we propose a simple one-parameter Padé’s approximation, which reproduces the exact Kohn-Sham surface kinetic energy over the entire range of metallic densities.
Ordered Phases in Cu2NiZn: A First-Principles Monte Carlo Study

Monte Carlo simulations based on effective interactions obtained from first-principles calculations reveal the existence of three ordered phases in ternary Cu2NiZn: (i) "modified"-L1(0) (0-600 K), (ii) L1(2) (600-850 K), and (iii) L1(0) (850-1200 K). This is in contrast to the generally accepted picture which assumes the existence of only two. We demonstrate that this sequence of phases is a consequence of the symmetry of the ground state and the magnitude of the dominating pair interactions. It agrees with available experimental data.

General information
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Organisations: Department of Physics, Theoretical Atomic-scale Physics, Uppsala University
Authors: Simak, S. (Ekstern), Ruban, A. (Intern), Abrikosov, I. (Ekstern), Skriver, H. L. (Intern), Johansson, B. (Ekstern)
Pages: 188-191
The energetics of steps on transition metal surfaces
The surface energy of metals
We have used density functional theory to establish a database of surface energies for low index surfaces of 60 metals in the periodic table. The data may be used as a consistent starting point for models of surface science phenomena. The accuracy of the database is established in a comparison with other density functional theory results and the calculated surface energy anisotropies are applied in a determination of the equilibrium shape of nano-crystals of Fe, Cu, Mo, Ta, Pt and Ph. (C) 1998 Elsevier Science B.V. All rights reserved.
Total energy calculations of random alloys: Supercell, Connolly-Williams and CPA methods

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Scopus rating (2007): SJR 0.682 SNIP 1.029
Scopus rating (2006): SJR 0.852 SNIP 1.474
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Scopus rating (2004): SJR 0.915 SNIP 1.06
Ab initio calculations of partial molar properties in the single-site approximation

We discuss the application of the single-site approximation in calculations of partial molar quantities, e.g., impurity solution energy, segregation energy, and effective chemical potential, which are related to a variation of the composition of an alloy or its nonequivalent parts. We demonstrate that these quantities may be considerably in error if they are obtained in methods based on the single-site approximation for fixed alloy compositions. This error does not reflect a breakdown but rather an inappropriate use of the single-site approximation which is, in fact, found to be sufficiently accurate when properly applied in calculations of partial molar quantities.
Ab initio full charge-density study of the atomic volume of α-phase Fr, Ra, Ac, Th, Pa, U, Np, and Pu
We have used a full charge-density technique based on the linear muffin-tin orbitals method in first-principles calculations of the atomic volumes of the light actinides including Fr, Ra, and Ac in their low-temperature crystallographic phases. The good agreement between the theoretical and experimental values along the series support the picture of itinerant 5f electronic states in Th to Pu. The increased deviation between theory and experiment found in Np and Pu may be an indication of correlation effects not included in the local density approximation.

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Authors: Vitos, L. (Intern), Kollár, J. (Ekstern), Skriver, H. L. (Intern)
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Anomalous atomic volume of alpha-Pu
We have performed full charge-density calculations for the equilibrium atomic volumes of the alpha-phase light actinide metals using the local density approximation (LDA) and the generalized gradient approximation (GGA). The average deviation between the experimental and the GGA atomic radii is 1.3%. The comparison between the LDA and GGA results show that the anomalously large atomic volume of alpha-Pu relative to alpha-Np can be ascribed to exchange-correlation effects connected with the presence of low coordinated sites in the structure where the f electrons are close to the onset of localization. This effect is correctly described in the GGA but not in the LDA.

General information
State: Published
Calculated site substitution in ternary gamma'-Ni3Al: Temperature and composition effects

The temperature and composition dependence of the site substitution behavior of ternary additions to Ni3Al is examined on the basis of first-principles calculations of the total energies of ternary, partially ordered (gamma') alloys. The calculations are performed by means of the linear muffin-tin orbitals method in conjunction with the local-density and multilattice coherent-potential approximations and include all 3d, 4d, 5d, and noble metals. The calculations show the existence of simple trends in the alloying behavior of the gamma' phase which may be explained in a Friedel-like model based on the interaction between Ni and the added species. It is shown that the commonly accepted interpretation of the site substitution behavior of Cu and Pd may be incorrect because of site substitution reversal at high temperatures. It is further shown that the direction of the solubility lobe in the ternary phase diagram for the elements Co, Pd, Cu, and Ag incorrectly has been interpreted as evidence for strong Ni site preference and that, in fact, these elements are expected to exhibit only weak Ni site preference.
Full charge-density scheme with a kinetic-energy correction: Application to ground-state properties of the 4d metals

We present a full charge-density technique to evaluate total energies from the output of self-consistent linear muffin-tin orbitals (LMTO) calculations in the atomic-sphere approximation (ASA). The Coulomb energy is calculated exactly from the complete, nonspherically symmetric charge density defined within nonoverlapping, space-filling Wigner-Seitz cells; the exchange-correlation energy is evaluated by means of the local-density approximation or the generalized gradient approximation applied to the complete charge-density; and the ASA kinetic energy is corrected for the nonspherically symmetric charge density by a gradient expansion. The technique retains most of the simplicity and the computational efficiency of the LMTO-ASA method, and calculations of atomic volumes and elastic constants of the 4d elements show that it has the accuracy of full-potential methods.
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.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Aarhus University
Authors: Murray, P. (Ekstern), Thorshaug, S. (Ekstern), Stensgaard, I. (Ekstern), Besenbacher, F. (Intern), Laegsgaard, E. (Ekstern), Ruban, A. (Intern), Jacobsen, K. W. (Intern), Kopidakis, G. (Intern), Skriver, H. L. (Intern)
Pages: 1380-1383
Publication date: 1997
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Review B Condensed Matter
Volume: 55
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BFI (2017): BFI-level 1
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BFI (2013): BFI-level 2
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 2
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BFI (2011): BFI-level 2
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BFI (2010): BFI-level 2

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Links:

Bibliographical note
Copyright (1997) by the American Physical Society.
Source: orbit
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Publication: Research - peer-review › Journal article – Annual report year: 1997
Locally self-consistent Green's function approach to the electronic structure problem

The locally self-consistent Green's function (LSGF) method is an order-N method for calculation of the electronic structure of systems with an arbitrary distribution of atoms of different kinds on an underlying crystal lattice. For each atom Dyson's equation is used to solve the electronic multiple scattering problem in a local interaction zone (LIZ) embedded in an effective medium judiciously chosen to minimize the size of the LIZ. The excellent real-space convergence of the LSGF calculations and the reliability of its results are demonstrated for a broad spectrum of metallic alloys with different degree of order. The relation of the convergence of our method to fundamental properties of the system, that is, the effective cluster interactions, is discussed.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Uppsala University
Authors: Abrikosov, I. (Ekstern), Simak, S. (Ekstern), Johansson, B. (Ekstern), Ruban, A. (Intern), Skriver, H. L. (Intern)
Publication date: 1997
Pages: 9319-9334
Main Research Area: Technical/natural sciences
Publication information
Journal: Physical Review B Condensed Matter
Volume: 56
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ISSN (Print): 0163-1829
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BFI (2016): BFI-level 2
BFI (2015): BFI-level 2
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BFI (2013): BFI-level 2
ISI indexed (2013): ISI indexed no
Magnetic properties of Fe embedded in V and Cr: Thin films and dilute alloys
We have calculated the magnetic moment of Fe as a function of the number of nearest V and Cr atoms. We find that the Fe magnetic moment disappears in a neighborhood of exclusively V atoms, but remains larger than 1.85 \( \mu_B \) in a Cr neighborhood. This behavior, which is in excellent agreement with experiment, is a result of the pseudogap formed in the bce state density.

General information
State: Published
Organisations: Theoretical Atomic-scale Physics, Department of Physics, Uppsala University
Authors: Mirbt, S. (Ekstern), Abrikosov, I. (Ekstern), Johansson, B. (Ekstern), Skriver, H. L. (Intern)
Pages: 67-69
Publication date: 1997
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Review B Condensed Matter
Volume: 55
Issue number: 1
ISSN (Print): 0163-1829
Ratings:

Electronic versions:
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DOI:
10.1103/PhysRevB.56.9319
Links:
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.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics
Authors: Christensen, A. (Intern), Ruban, A. (Intern), Stoltze, P. (Intern), Jacobsen, K. W. (Intern), Skriver, H. L. (Intern), Nørskov, J. K. (Intern), Besenbacher, F. (Intern)
Pages: 5822-5834
Publication date: 1997
Main Research Area: Technical/natural sciences

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Journal: Physical Review B Condensed Matter
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- BFI (2017): BFI-level 1
- BFI (2016): BFI-level 2
- BFI (2015): BFI-level 2
- BFI (2014): BFI-level 2
- BFI (2013): BFI-level 2
- ISI indexed (2013): ISI indexed no
- BFI (2012): BFI-level 2
- ISI indexed (2012): ISI indexed no
- BFI (2011): BFI-level 2
- ISI indexed (2011): ISI indexed no
- BFI (2010): BFI-level 2
- BFI (2009): BFI-level 2
- BFI (2008): BFI-level 2
Original language: English

Electronic versions:
- Ruban.pdf

Links:

Bibliographical note
Copyright (1997) by the American Physical Society.
Quantum-well-induced ferromagnetism in thin films

We have used a first-principles Green's-function technique to investigate the magnetic properties of thin films of Rh, Pd, and Pt deposited on a fee Ag (001) substrate. We find that the magnetic moment of the film is periodically suppressed and enhanced as a function of film thickness. The phenomenon is explained in terms of quantum-well states moving through the Fermi level with increasing film thickness.

Surface electronic structure and reactivity of transition and noble metals

Surface electronic structure and reactivity of transition and noble metals

Magnetic, states, Rh, Ru, 4D, metal overlays, Pd, surfaces, Green-function, substrate
Surface, segregation profile for Ni50Pd50(100)
A recent dynamical LEED study [G.N. Derry, C.B. McVey, P.J. Rous, Surf. Sci. 326 (1995) 59] reported an oscillatory surface segregation profile in the Ni50Pd50(100) system with the surface layer enriched by Pd. We have performed ab-initio total-energy calculations for the surface of this alloy system using the coherent potential approximation and obtain an oscillatory segregation profile, in agreement with experiments. We discuss the energetic origin of the oscillatory segregation profile in terms of effective cluster interactions. We include relaxation effects by means of the semi-empirical effective medium theory, and find that this cannot explain the remaining differences between theory and experiment. (C) 1997 Elsevier Science B.V.

General information
State: Published
Organisations: Department of Physics
Authors: Christensen, A. (Intern), Ruban, A. (Intern), Skrøver, H. L. (Intern)
Pages: 235-240
Publication date: 1997
Main Research Area: Technical/natural sciences
We have performed an ab initio study of the oscillation periods of the interlayer coupling in sandwiches of [100] layers of body centered cubic Cr, respectively, Mo, with up to 20 monolayers thickness embedded in an Fe host. Our derived values for the oscillation periods of the interlayer coupling agree well with those expected from the respective Fermi surface calipers and are in excellent agreement with experiment. We compare the interlayer coupling across a nonenhanced paramagnetic Cr spacer with the interlayer coupling across a Cr spacer in the spin-density wave state. We find that the spin-density wave gives rise to an additional contribution to the interlayer coupling. The origin of the observed and calculated 18 Ångstrom period of the interlayer coupling can be explained as due to a caliper of the Fermi surface of Cr in the CsCl structure. In the case of the Mo spacer we investigate the influence of the lattice constant on the interlayer coupling and also the dependence of the interlayer coupling amplitude on the Fe magnetic moment.
Determination of the electronic density of states near buried interfaces: Application to Co/Cu multilayers

High-resolution L(3) x-ray absorption and emission spectra of Co and Cu in Co/Cu multilayers are shown to provide unique information on the occupied and unoccupied density of d states near buried interfaces. The d bands of both Co and Cu interfacial layers are shown to be considerably narrowed relative to the bulk metals, and for Cu interface layers the d density of states is found to be enhanced near the Fermi level. The experimental results are confirmed by self-consistent electronic structure calculations.

General information
State: Published
Organisations: Theoretical Atomic-scale Physics, Department of Physics, Uppsala University, IBM Research GmbH
Authors: Nilsson, A. (Ekstern), Sthör, J. (Ekstern), Wiell, T. (Ekstern), Aldén, M. (Ekstern), Bennich, P. (Ekstern), Wassdahl, N. (Ekstern), Samant, M. (Ekstern), Parkin, S. (Ekstern), Mårtensson, N. (Ekstern), Nordgren, J. (Ekstern), Johansson, B. (Ekstern), Skriver, H. L. (Intern)
Pages: 2917-2921
Publication date: 1996
Main Research Area: Technical/natural sciences

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Volume: 54
Issue number: 4
ISSN (Print): 1098-0121
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BFI (2017): BFI-level 2
BFI (2016): BFI-level 2
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.933 SNIP 0.94
BFI (2014): BFI-level 2
We present an ab initio determination of the crystallographic phase stability of Fe-Co alloys as a function of concentration, using the coherent potential approximation. A bcc --> hcp phase transition is found at a concentration of 85 at.% of Co, in good agreement with the experimental phase diagram. We demonstrate that for the Fe-rich random alloys magnetism-stabilizes the bcc phase relative to the close-packed fee and hcp phases. Magnetism also favors the partially ordered alpha' phase relative to the random bcc alloy. This unique relation between magnetism and phase stability for the Fe-Co alloys is analyzed by a spin-polarized canonical d-band model.
Order- N Green's Function Technique for Local Environment Effects in Alloys
We have developed a new approach to the calculations of ground state properties of large crystalline systems with arbitrary atomic configurations based on a Green's function technique in conjunction with a self-consistent effective medium for the underlying randomly occupied lattice. The locally self-consistent multiple scattering method and the coherent potential approximation are two simple limits of our general formulation. The efficiency and the excellent convergence properties of the method are demonstrated in calculations for two alloy systems, Cu-Zn and Rh-Pd.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Uppsala University
Authors: Abrikosov, I. A. (Ekstern), Niklasson, A. M. N. (Ekstern), Simak, S. I. (Ekstern), Johansson, B. (Ekstern), Ruban, A. (Intern), Skriver, H. L. (Intern)
Pages: 4203-4206
Publication date: 1996
Main Research Area: Technical/natural sciences

Publication Information
Journal: Physical Review Letters
Volume: 76
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ISSN (Print): 0031-9007
Ratings:
BFI (2017): BFI-level 2
BFI (2016): BFI-level 2
Scopus rating (2016): SJR 3.56 SNIP 2.133
BFI (2015): BFI-level 2
Quantum-well-driven magnetism in thin films
We have performed local spin-density calculations for an fcc (100) Ag substrate covered by 1 to 16 monolayers (ML) of Pd. We find that thin films of Pd are magnetic with a moment of the order of 0.3 μB except for films of 1-2 ML and 5-7 ML where magnetism is completely suppressed. We present a physically transparent explanation of this behavior in terms of the Stoner picture and magnetic quantum-well states.
Quantum-well states and induced magnetism in Fe/CuN/Fe bcc (001) trilayers

We have used a first-principles Green's function technique to investigate the formation of magnetic moments in Fe/CuN/Fe bcc (001) trilayers. We show that the magnetic moment in the paramagnetic spacer material to a first approximation may be described as a linear superposition of the magnetic profiles of two single Fe/Cu interfaces. The small deviations from this simple superposition are shown to be a consequence of quantum-well states confined within the paramagnetic spacer. This connection is confirmed by direct calculation of the state density. The results are of conceptual interest for the understanding of the exchange coupling.
Calculated Phase Diagram for the $\gamma \leftrightarrow \alpha$ Transition in Ce

We have calculated the pressure-temperature phase diagram of the $\gamma \leftrightarrow \alpha$ isostructural transition in Ce on the basis of the Mott transition model. The theory correctly describes the linear variation of the transition temperature with pressure and the existence of a critical point. The quantitative agreement with the experimental diagram is good. The influence of different free energy contributions (configurational, magnetic, and vibrational) on the phase transition in Ce is discussed.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Uppsala University
Authors: Johansson, B. (Ekstern), Abrikosov, I. A. (Ekstern), Aldén, M. (Ekstern), Ruban, A. (Intern), Skriver, H. L. (Intern)
Publication date: 1995
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Review Letters
Volume: 74
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BFI (2017): BFI-level 2
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Scopus rating (2016): SJR 3.56 SNIP 2.133
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Scopus rating (2015): SJR 3.823 SNIP 2.205
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 5.027 SNIP 2.646
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 5.674 SNIP 2.796
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 6.252 SNIP 2.886
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2

Calculated Phase Diagram for the $\gamma \leftrightarrow \alpha$ Transition in Ce

We have calculated the pressure-temperature phase diagram of the $\gamma \leftrightarrow \alpha$ isostructural transition in Ce on the basis of the Mott transition model. The theory correctly describes the linear variation of the transition temperature with pressure and the existence of a critical point. The quantitative agreement with the experimental diagram is good. The influence of different free energy contributions (configurational, magnetic, and vibrational) on the phase transition in Ce is discussed.
Ground-state properties of ordered, partially ordered, and random Cu-Au and Ni-Pt alloys

We have studied the ground-state properties of ordered, partially ordered, and random Cu-Au and Ni-Pt alloys at the stoichiometric 1/4, 1/2, and 3/4 compositions in the framework of the multisublattice single-site (SS) coherent potential approximation (CPA). Charge-transfer effects in the random and the partially ordered alloys are included in the screened impurity model. The prefactor in the Madelung energy is determined by the requirement that the total energy obtained in direct SS CPA calculations should equal the total energy given by the Connolly-Williams expansion based on Green’s function calculations for the ordered alloys that do not rely on the single-site approximation. We find that the prefactor to a large degree is independent of a lattice constant, concentration, and a long-range-order parameter and may be considered constant for a given alloy system. The calculated heats of formation for the ordered alloys are in good agreement with experimental data. For all the alloys the calculated ordering energy and the equilibrium lattices parameters are found to be almost exact quadratic functions of the long-range-order parameter.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Uppsala University
Authors: Ruban, A. (Intern), Abrikosov, I. A. (Ekstern), Skriver, H. L. (Intern)
Pages: 12958-12968
Publication date: 1995
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Review B Condensed Matter
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ISSN (Print): 0163-1829
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BFI (2017): BFI-level 1
BFI (2016): BFI-level 2
BFI (2015): BFI-level 2
BFI (2014): BFI-level 2
Madelung energy for random metallic alloys in the coherent potential approximation

Within the conventional single-site coherent potential approximation (CPA) used to calculate thermodynamic properties of random alloys, the effect of charge transfer is neglected. We discuss a number of recent models based on the same mathematical form but with a different prefactor $\beta$ which allow one to include charge-transfer effects in the framework of the CPA. We show how the models work in actual calculations for selected metallic alloy systems, Al-Li, Li-Mg, and Ni-Pt, which exhibit charge transfer. We find that the so-called screened impurity model ($\beta=1$), which is derived completely within the mean-field single-site approximation, leads to the best agreement with experimental lattice parameter and mixing energy data for Al-Li and Li-Mg alloys. However, for the Ni-Pt system exhibiting strong ordering tendency this model seems to overestimate the Madelung energy of the completely random alloy, and in this case the screened-CPA method ($\beta=1/2$) gives more correct results. It is suggested that a comparison with the results obtained by the Connolly-Williams method may be used to determine an optimal value for $\beta$ depending on the alloy under consideration.

General information

State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Uppsala University
Authors: Korzhavyi, P. A. (Ekstern), Ruban, A. (Intern), Abrikosov, I. A. (Ekstern), Skriver, H. L. (Intern)
Pages: 5773-5780
Publication date: 1995
Main Research Area: Technical/natural sciences

Publication information

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BFI (2017): BFI-level 1
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BFI (2015): BFI-level 2
BFI (2014): BFI-level 2
BFI (2013): BFI-level 2
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 2
ISI indexed (2012): ISI indexed no
Magnetic coupling in 3d transition-metal monolayers and bilayers on bcc (100) iron

We have calculated the magnetization profile in the (100) surface of bcc Fe covered by a monolayer or a bilayer of 3d transition metals. The calculated trends are explained in terms of the hybridization between the 3d states of the overlayer and the Fe substrate.

General information
State: Published
Organisations: Theoretical Atomic-scale Physics, Department of Physics, Uppsala University
Authors: Mirbt, S. (Ekstern), Eriksson, O. (Ekstern), Johansson, B. (Ekstern), Skriver, H. L. (Intern)
Pages: 15070-15073
Publication date: 1995
Main Research Area: Technical/natural sciences

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BFI (2014): BFI-level 2
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ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 2
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 2
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 2
BFI (2009): BFI-level 2
BFI (2008): BFI-level 2
Original language: English
ELECTRONIC-STRUCTURE, FE(001), INTERFACE MAGNETISM, SURFACE MAGNETISM, COBALT, LAYERS, FE(100)
Electronic versions:
Mirbt.pdf
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10.1103/PhysRevB.52.15070
Origin of metallic surface core-level shifts
The unique property of the open 4f energy shell in the lanthanide metals is used to show that the initial-state energy shift gives an insufficient description of surface core-level shifts. Instead a treatment, which fully includes the final-state screening, account for the experimentally observed surface shifts of the occupied as well as the unoccupied 4f states. The surface energy shift of the initial state corresponds approximately to the average of the shifts for the occupied and unoccupied 4f levels.

General information
State: Published
Organisations: Theoretical Atomic-scale Physics, Department of Physics, Cap Programator, Uppsala University
Authors: Aldén, M. (Ekstern), Skriver, H. L. (Intern), Abrikosov, I. A. (Ekstern), Johansson, B. (Ekstern)
Pages: 1981-1984
Publication date: 1995
Main Research Area: Technical/natural sciences
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ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 2
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 2
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 2
BFI (2009): BFI-level 2
BFI (2008): BFI-level 2
Original language: English
STATES, RARE-EARTH-METALS, DENSITY, ELEMENTS, SEGREGATION, BINDING-ENERGY SHIFTS
Electronic versions:
Alden.pdf
DOIs:
Links:

Surface shift of the occupied and unoccupied 4f levels of the rare-earth metals
The surface energy shifts of the occupied and unoccupied 4f levels for the lanthanide metals have been calculated from first principles by means of a Green’s-function technique within the tight-binding linear muffin-tin orbitals method. We use the concept of complete screening to identify the occupied and unoccupied 4f energy level shifts as the surface...
segregation energy of a 4fn-1 and 4fn+1 impurity atom, respectively, in a 4fn host metal. The calculations include both initial- and final-state effects and give values that are considerably lower than those measured on polycrystalline samples as well as those found in previous initial-state model calculations. The present theory agrees well with very recent high-resolution, single-crystal film measurements for Gd, Tb, Dy, Ho, Er, Tm, and Lu. We furthermore utilize the unique possibility offered by the lanthanide metals to clarify the roles played by the initial and the different final states of the core-excitation process, permitted by the fact that the so-called initial-state effect is identical upon 4f removal and 4f addition. Surface energy and work function calculations are also reported.

General information
State: Published
Organisations: Theoretical Atomic-scale Physics, Department of Physics, Uppsala University
Authors: Aldén, M. (Ekstern), Johansson, B. (Ekstern), Skriver, H. L. (Intern)
Pages: 5386-5396
Publication date: 1995
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Review B Condensed Matter
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BFI (2012): BFI-level 2
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BFI (2011): BFI-level 2
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BFI (2010): BFI-level 2
BFI (2009): BFI-level 2
BFI (2008): BFI-level 2
Original language: English
LAYER, VALENCE STATE, SEGREGATION ENERGIES, DENSITY, INTERFACES, CRYSTALS, ELEMENTAL METALS, SAMARIUM METAL, WORK FUNCTION, GREEN-FUNCTION
Electronic versions:
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DOIs:
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Links:

Bibliographical note
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Source: orbit
Source-ID: 252052
Publication: Research - peer-review › Journal article – Annual report year: 1995

Theoretical aspects of the FecNi1-c Invar alloy
We present first-principles coherent-potential-approximation calculations for the fcc FeNi alloy. We have found that this system is characterized by a competition between a low-spin (LS) and a high-spin (HS) state, and we have calculated this energy difference as a function of alloy concentration. For fcc Fe we find that several magnetic states are locally stable whereas for the FeNi alloys only one magnetic state is stable. In agreement with previous theories for explaining the Invar effect in the Fe65Ni35 alloy, we find that at this concentration the LS and HS states are very similar in energy. The calculated magnetic moment, equilibrium volume, and bulk modulus agree well with experimental data, and we predict that the Grüneisen constant exhibits an anomaly at a Ni concentration around 25%.

General information
State: Published
Ab initio study of antiphase boundaries and stacking faults in L1₂ and DO₂₂ compounds

We have performed ab initio calculations of the energies of antiphase boundaries as well as complex and superlattice intrinsic stacking faults in nine intermetallic compounds observed in the face-centered-cubic L₁₂ and DO₂₂ structures. The calculations were performed by means of a Green's function technique based on the linear-muffin-tin-orbitals method within the tight-binding and atomic-sphere approximations.
Ab initio study of long-period superstructures in close-packed A3B compounds
We have performed ab initio calculations of the stability of one-dimensional long-period superstructures in Cu3Pd, Cu3Al, and Ag3Mg by means of an interface Green's function technique based on the linear-muffin-tin-orbitals method within the tight-binding and atomic-sphere approximations. The energies of the superstructures relative to the L1(2) structure are found by an expansion based on the calculated energy of a single (001) antiphase boundary and the calculated interaction energy between two and three antiphase boundaries of varying distance. The expansion agrees with standard band-structure calculations of the structural energy differences for the two short-period superstructures DO22 and DO23. We find that at zero temperature the ground states of Cu3Pd, Cu3Al, and Ag3Mg are one-dimensional superstructures with antiphase boundary separations of 2-5 unit cells of the underlying L1(2) structure.
Calculated orientation dependence of surface segregations in Pt50Ni50

We present local-density calculations of surface segregation profiles in a random Pt50Ni50 alloy. We find that the concentration profiles of the three low-index surfaces oscillate and that the two most closely packed surfaces, i.e., (111) and (100), are enriched by Pt while Ni is found to segregate to the surface of the (110) face. These results may be explained in terms of a competition between the tendency of Pt to segregate towards the two first surface layers at the (110) face and the tendency to form a structure of alternating Pt and Ni layers.
We have calculated the surface energy and the work function of the 4d metals by means of an energy functional based on a self-consistent, spherically symmetric atomic-sphere potential. In this approach the kinetic energy is calculated completely within the atomic-sphere approximation (ASA) by means of a spherically symmetrized charge density, while the Coulomb and exchange-correlation contributions are calculated by means of the complete, nonspherically symmetric charge density within nonoverlapping, space-filling Wigner-Seitz cells. The functional is used to assess the convergence and the accuracy of the linear-muffin-tin-orbitals (LMTO) method and the ASA in surface calculations. We find that the full charge-density functional improves the agreement with recent full-potential LMTO calculations to a level where the average deviation in surface energy over the 4d series is down to 10%.
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
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Organisations: Theoretical Atomic-scale Physics, Department of Physics, Uppsala University, Moscow Institute for Steel and Alloys
Authors: Ruban, A. (Intern), Abrikosov, I. A. (Ekstern), Kats, D. Y. (Ekstern), Gorelikov, D. (Ekstern), Jacobsen, K. W. (Intern), Skriver, H. L. (Intern)
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Self-consistent Green's-function technique for bulk and surface impurity calculations: Surface core-level shifts by complete screening
We have implemented an efficient self-consistent Green's-function technique, based on the tight-binding linear-muffin-tin-orbitals method, for calculating the electronic structure and total energy of a substitutional impurity located either in the bulk or at the surface. The technique makes use of the frozen-core and atomic-sphere approximation but, in addition, includes the dipole contribution to the intersphere potential. Within the concept of complete screening, we identify the surface core-level binding-energy shift with the surface segregation energy of a core-ionized atom and use the Green's-
function impurity technique in a comprehensive study of the surface core-level shifts (SCLS) of the 4d and 5d transition metals. In those cases, where observed data refer to single crystals, we obtain good agreement with experiment, whereas the calculations typically underestimate the measured shift obtained from a polycrystalline surface. Comparison is made with independent theoretical data for the surface core-level eigenvalue shift, and the much debated role of the so-called initial-and final-state contributions to the SCLS is discussed.

**General information**

State: Published
Organisations: Theoretical Atomic-scale Physics, Department of Physics, Uppsala University, Technical University of Denmark
Authors: Aldén, M. (Ekstern), Abrikosov, I. A. (Ekstern), Johansson, B. (Ekstern), Rosengaard, N. M. (Ekstern), Skriver, H. L. (Intern)
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**Surface core-level shifts for simple metals**

We have performed an ab initio study of the surface core-level binding energy shift (SCLS) for 11 of the simple metals by means of a Green’s-function technique within the tight-binding linear-muffin-tin-orbitals method. Initial- and final-state effects are included within the concept of complete screening, whereby a SCLS becomes equivalent to the surface segregation energy of a core-ionized atom, a quantity we obtain by separate bulk and surface impurity calculations. The results are in good agreement with experiment in most of those cases where the data originates from single-crystal measurements. We discuss the surface shifts of the electrostatic potentials and the band centers in order to trace the microscopic origin of the SCLS in the simple metals and find that the anomalous subsurface core-level shifts in beryllium are caused by charge dipoles, which persist several layers into the bulk. We furthermore conclude that the unexpected negative sign of the SCLS in beryllium is predominantly an initial-state effect and is caused by the high electron density in this metal.
Surface energy and work function of the light actinides

We have calculated the surface energy and work function of the light actinides Fr, Ra, Ac, Th, Pa, U, Np, and Pu by means of a Green's-function technique based on the linear-muffin-tin-orbitals method within the tight-binding representation. In these calculations we apply an energy functional which combines the kinetic energy calculated within the atomic-sphere approximation with Coulomb- and exchange-correlation-energy terms calculated by means of the complete nonspherically symmetric charge density derived from the atomic-sphere potential within nonoverlapping and space-filling cells. The calculated surface energies and work functions are in good agreement with the limited experimental data.

General information
State: Published
Organisations: Theoretical Atomic-scale Physics, Department of Physics, Research Institute for Solid State Physics
Authors: Kollár, J. (Ekstern), Vitos, L. (Intern), Skriver, H. L. (Intern)
Pages: 11288-11292
Publication date: 1994
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Review B Condensed Matter
Ab initio surface core-level shifts and surface segregation energies

We have calculated the surface core-level energy shifts of the 4d and 5d transition metals by means of local-density theory and a Green’s-function technique based on the linear muffin-tin orbitals method. Final-state effects are included by treating the core-ionized atom as an impurity located in the bulk and at the surface, respectively. It is shown that the study of surface core-level shifts provides an ideal tool for an accurate determination of the surface segregation energy of a substitutional (Z+1) impurity in a Z metal host (Z denotes atomic number).
Calculated stacking-fault energies of elemental metals

We have performed ab initio calculations of twin, intrinsic, and extrinsic face-centered-cubic stacking faults for all the 3d, 4d, and 5d transition metals by means of a Green's-function technique, based on the linear-muffin-tin-orbitals method within the tight-binding and atomic-sphere approximations. The results are in excellent agreement with recent layer Korringa-Kohn-Rostoker Green's-function calculations where stacking-fault energies for Ni, Cu, Rh, Pd, Ag, Ir, and Au were found by means of the the so-called force theorem. We find that the self-consistent fault energies for all the metals in the three transition series vary with atomic number essentially as the calculated structural energy differences between the face-centered-cubic and the hexagonal-close-packed phases. In addition we find that the simple relationships between the different types of fault energies predicted by models based on the local atomic coordination are obeyed to a high degree of accuracy.

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Organisations: Theoretical Atomic-scale Physics, Department of Physics, Technical University of Denmark
Authors: Rosengaard, N. M. (Ekstern), Skriver, H. L. (Intern)
Pages: 12865-12873
Publication date: 1993
Main Research Area: Technical/natural sciences
Deep layer-resolved core-level shifts in the beryllium surface

Core-level energy shifts for the beryllium surface region are calculated by means of a Green's function technique within the tight-binding linear muffin-tin orbitals method. Both initial- and final-state effects in the core-ionization process are fully accounted for. Anomalously large energy shifts are found for the three topmost surface layers in agreement with recent experimental data. The reason for this extraordinary behavior is explained.
Self-consistent linear-muffin-tin-orbitals coherent-potential technique for bulk and surface calculations: Cu-Ni, Ag-Pd, and Au-Pt random alloys

We present an efficient technique for calculating surface properties of random alloys based on the coherent-potential approximation within a tight-binding linear-muffin-tin-orbitals basis. The technique has been applied in the calculation of bulk thermodynamic properties as well as (001) surface energies and work functions for three fcc-based alloys (Cu-Ni, Ag-Pd, and Au-Pt) over the complete concentration range. The calculated mixing enthalpies for the Ag-Pd and Au-Pt systems agree with experimental values, and the calculated concentration dependence of the lattice parameters agrees with experiment for all three systems. We find that the calculated surface energies and work functions in the unsegregated case exhibit a small positive deviation from a linear concentration dependence. Finally, we performed a segregation analysis based on the calculated surface energies by means of a simple thermodynamic model and found in complete agreement with experiment that the noble metals segregate strongly towards the surface of their alloys.
Ab initio work function of elemental metals

We have used a recently developed self-consistent Green’s-function technique based on tight-binding linear-muffin-tin-orbital theory to calculate the work function for the close-packed surfaces of 37 elemental metals. The results agree with the limited experimental data obtained from single crystals to within 15%, and they explain the smooth behavior of the polycrystalline data as a function of atomic number.
Calculated surface-energy anomaly in the 3d metals

Local-spin-density theory and a Green’s-function technique based on the linear muffin-tin orbitals method have been used to calculate the surface energy of the 3d metals. The theory explains the variation of the values derived from measurements of the surface tension of liquid metals including the pronounced anomaly occurring between vanadium and nickel in terms of a decrease in the d contribution caused by spin polarization.

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Organisations: Theoretical Atomic-scale Physics, Department of Physics
Authors: Aldén, M. (Ekstern), Skriver, H. L. (Intern), Mirbt, S. (Ekstern), Johansson, B. (Ekstern)
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Main Research Area: Technical/natural sciences

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BFI (2014): BFI-level 2
Scopus rating (2014): SJR 5.027 SNIP 2.646
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 5.674 SNIP 2.796
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ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 6.252 SNIP 2.886
Surface energy and work function of elemental metals

We have performed an ab initio study of the surface energy and the work function for six close-packed surfaces of 40 elemental metals by means of a Green's-function technique, based on the linear-muffin-tin-orbitals method within the tight-binding and atomic-sphere approximations. The results are in excellent agreement with a recent full-potential, all-electron, slab-supercell calculation of surface energies and work functions for the 4d metals. The present calculations explain the trend exhibited by the surface energies of the alkali, alkaline earth, divalent rare-earth, 3d, 4d, and 5d transition and noble metals, as derived from the surface tension of liquid metals. In addition, they give work functions which agree with the limited experimental data obtained from single crystals to within 15%, and explain the smooth behavior of the experimental work functions of polycrystalline samples as a function of atomic number. It is argued that the surface energies and work functions calculated by present day ab initio methods are at least as accurate as the experimental values.

General information
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Organisations: Theoretical Atomic-scale Physics, Department of Physics, Technical University of Denmark
Authors: Skriver, H. L. (Intern), Rosengaard, N. M. (Ekstern)
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Surface magnetism in iron, cobalt, and nickel

We have calculated magnetic moments, work functions, and surface energies for several of the most closely packed surfaces of iron, cobalt, and nickel by means of a spin-polarized Green’s-function technique based on the linear muffin-tin orbitals method within the tight-binding and atomic sphere approximations. We find enhanced spin moments at all the surfaces considered except for Ni fcc(111), where the moment at the surface reverts to its bulk value. This is in close agreement with earlier slab calculations. In addition, we find that the calculated work functions and surface energies agree with experimental values to within 10%, which may be considered most satisfactory in view of the computational efficiency of the Green’s function technique. Exchange and correlation have been treated within the local spin-density approximation and we have considered three different parametrizations of the original many-body data. We find that the calculated work functions depend as much on the choice of this parametrization as on the effect of spin polarization.
Self-consistent Green's-function technique for surfaces and interfaces

We have implemented an efficient self-consistent Green's-function technique for calculating ground-state properties of surfaces and interfaces, based on the linear-muffin-tin-orbitals method within the tight-binding representation. In this approach the interlayer interaction is extremely short ranged, and only a few layers close to the interface need be treated self-consistently via a Dyson equation. For semi-infinite jellium, the technique gives work functions and surface energies that are in excellent agreement with earlier calculations. For the bcc(110) surface of the alkali metals, we find surface energies in close agreement with values derived from surface tensions of the liquid metals, and work functions that deviate less than 10% from the experimental values.
Electron-phonon coupling in the rare-earth metals

We have estimated the strength of the mass enhancement of the conduction electrons due to electron-phonon interaction in the rare metals Sc, Y, and La–Lu. The underlying self-consistent energy bands were obtained by means of the scalar relativistic linear-muffin-tin-orbital method, and the electron-phonon parameters were calculated within the Gaspari-Gyorffy formulation. For the heavier rare earths Gd–Tm spin polarization was included both in the band-structure calculations and in the treatment of the electron-phonon coupling to take into account the spin splitting of the conduction electrons induced by the 4f states. The calculated electron-phonon mass enhancement $\lambda$ exhibits a pronounced variation through the series with a maximum value of 1.07 in Pr and a minimum of 0.3 in Ho. We analyze the experimental data from specific heat and de Haas–van Alphen measurements in light of the calculated electron-phonon contribution to the mass enhancement. Finally, we present for the superconducting elements Sc, Y, La, and Lu a comparison with the empirical electron-phonon coupling constants derived from the transition temperatures.
Electronic structure and magnetic properties of selected lanthanide and actinide intermetallic Laves-phase alloys
The electronic structure and magnetic properties of some yttrium and uranium Laves-phase pseudobinary alloys with 3d elements have been calculated. The calculations were done by simulating the electronic structure of the alloy by that of an ordered compound with the same stoichiometry. In general a good agreement between the experimental and theoretical magnetic moment was found, indicating that the spurious long-range order of the calculations is of minor importance. A comparison between the present supercell cluster approach and the virtual-crystal approximation for the electronic structure and cohesive properties is presented for Y(Fe0.75Co0.25)2 and U(Fe0.5Ni0.5)2.

General information
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Organisations: Theoretical Atomic-scale Physics, Department of Physics, Uppsala University
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Electronic structure, cohesive, and magnetic properties of the actinide-iridium Laves phases
The electronic structure of the isostructural AIr2 systems (A=Th, Pa, U, Np, Pu, and Am) has been obtained by means of the scalar relativistic and fully relativistic linear muffin-tin orbital techniques. Ground-state properties such as lattice constants and onset of magnetic order have been calculated and compared with measured data. The hybridization between the actinide 5f and the ligand 5d states and the direct 5f wave-function overlap are found to be of comparable importance for the bandwidth of the itinerant 5f states. The anomalous paramagnetism of PuIr2 can be explained only by a fully relativistic treatment.

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Organisations: Theoretical Atomic-scale Physics, Department of Physics
Authors: Eriksson, O. (Ekstern), Johansson, B. (Ekstern), Brooks, M. S. S. (Ekstern), Skriver, H. L. (Intern)
Pages: 5647-5654
Electronic structure of the actinide-Rh3 systems and the 5f localization in UPd3

We present electronic-structure calculations for the isostructural (AuCu3-structure) series of intermetallic compounds ARh3 (A=Ac, Th, Pa, U, Np, Pu, Am, and Cm). The calculations were performed using both the scalar relativistic and the fully relativistic linear muffin-tin orbital (LMTO) method. Calculated cohesive and magnetic properties are compared with available experimental data. The onset of magnetism is discussed by means of a relativistic Stoner theory. The influence of the ligand states on the uranium 5f electrons is studied for the UM3 (M=Mo, Tc, Ru, Rh, Pd, and Ag) series of compounds. The localization of the 5f electrons in UPd3 as opposed to the itinerant 5f behavior for the earlier compounds (UMo3, UTC3 , URu3, and URh3) is explained in terms of the variation of the hybridization between 5f and ligand 4d states through the series.

Electronic structure of the actinide-Rh3 systems and the 5f localization in UPd3

We present electronic-structure calculations for the isostructural (AuCu3-structure) series of intermetallic compounds ARh3 (A=Ac, Th, Pa, U, Np, Pu, Am, and Cm). The calculations were performed using both the scalar relativistic and the fully relativistic linear muffin-tin orbital (LMTO) method. Calculated cohesive and magnetic properties are compared with available experimental data. The onset of magnetism is discussed by means of a relativistic Stoner theory. The influence of the ligand states on the uranium 5f electrons is studied for the UM3 (M=Mo, Tc, Ru, Rh, Pd, and Ag) series of compounds. The localization of the 5f electrons in UPd3 as opposed to the itinerant 5f behavior for the earlier compounds (UMo3, UTC3 , URu3, and URh3) is explained in terms of the variation of the hybridization between 5f and ligand 4d states through the series.

Electronic structure of the actinide-Rh3 systems and the 5f localization in UPd3

We present electronic-structure calculations for the isostructural (AuCu3-structure) series of intermetallic compounds ARh3 (A=Ac, Th, Pa, U, Np, Pu, Am, and Cm). The calculations were performed using both the scalar relativistic and the fully relativistic linear muffin-tin orbital (LMTO) method. Calculated cohesive and magnetic properties are compared with available experimental data. The onset of magnetism is discussed by means of a relativistic Stoner theory. The influence of the ligand states on the uranium 5f electrons is studied for the UM3 (M=Mo, Tc, Ru, Rh, Pd, and Ag) series of compounds. The localization of the 5f electrons in UPd3 as opposed to the itinerant 5f behavior for the earlier compounds (UMo3, UTC3 , URu3, and URh3) is explained in terms of the variation of the hybridization between 5f and ligand 4d states through the series.
Itinerant magnetism in CeRh₃B₂

Spin-polarized energy-band calculations, including spin-orbit coupling in the band Hamiltonian, have been performed on CeRh₃B₂. Good agreement is obtained between theory and experiment concerning the magnetic moment. It is also found that the magnetic moment varies strongly with volume and from this a qualitative explanation for the anomalously high Curie temperature of the compound is proposed. Furthermore, the spin density is found to be highly nonspherical.
A New High Pressure Phase and the Equation of State of YbH$_2$

High-pressure X-ray diffraction studies have been performed on YbH$_2$ up to 28 GPa. A first order phase transition from an orthorhombic structure to a collapsed hexagonal structure with $c/a = 1.34$ has been observed at about 15 GPa. The transition is accompanied by a 5.2% decrease in volume. Fitting the $V(P)$ data to Murnaghan's equation of state yields the bulk modulus $B_0 = 40.2$ GPa and its pressure derivative $B'_0 = 4.75$ for the orthorhombic phase. For the hexagonal phase we find the bulk modulus to be $B = B_0 = 138$ GPa independent of pressure, i.e. $B'_0 = 0$.

Electronic Structure and Bulk Ground State Properties of the Actinides

General information
One-Electron Theory of Metals. Cohesive and Structural Properties

The work described in the report and the 16 accompanying publications is based upon a one-electron theory obtained within the local approximation to density-functional theory, and deals with the ground state of metals as obtained from selfconsistent electronic-structure calculations performed by means of the Linear Muffin-Tin Orbital (LMTO) method. It has been the goal of the work to establish how well this one-electron approach describes physical properties such as the crystal structures of the transition metals, the structural phase transitions in the alkali, alkaline earth, and rare earth metals, and the localization of 3d, 4f, and 5f electrons in the 3d metal monoxides, the light lanthanides, and the actinides, respectively, as well as the cohesive properties of metals in general.

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Authors: Skriver, H. L. (Intern)
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Authors: Skriver, H. L. (Intern)
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Lattice Dynamics of fcc Ca
A large single crystal of FCC Ca was grown and was used to study the lattice dynamics of this divalent metal by coherent inelastic neutron scattering. The phonon dispersion curves were measured, at room temperature, along the [ξ00], [ξξ0], [ξξξ], and [0ξ1] symmetry directions. The dispersion curves bear a striking resemblance to those of FCC Yb, which is also a divalent metal with an electronic band structure similar to that of Ca. In particular, the shear moduli c44 and (c11-c 12)/2 differ by a factor of 3.4, which implies that FCC Ca (like FCC Yb) is very anisotropic with regard to the propagation of elastic waves. The frequencies of the T1[ξξ0] branch for ξ between approximately 0.5 and 0.8 are slightly above the velocity-of-sound line determined from the low-frequency measurements. Since a similar effect has been observed in FCC Yb, it is natural to assume that the anomalous dispersion exhibited by the T1 [ξξ0] branches of these metals is due to an electronic effect. To provide further support for this assumption the authors have performed a band theoretical calculation of the generalized susceptibility χ(q=0) of FCC Ca. The results suggest that, for ξ between approximately 0.6 and 0.8, there is a relative decrease in the electronic screening of the vibrational motion of the nuclei, which may account for the positive dispersion exhibited by the T1 [ξξ0] branch in this range of ξ values. The data were used to evaluate the elastic constants, the phonon density of states, and the lattice specific heat of FCC Ca.

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Organisations: Risø National Laboratory for Sustainable Energy
Authors: Stassis, C. (Ekstern), Zaretsky, J. (Ekstern), Misemer, D. K. (Ekstern), Skriver, H. L. (Intern), Harmon, B. (Ekstern)
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Electronic Structure of the Actinide Metals

Some recent experimental photoelectron spectroscopic results for the actinide metals are reviewed and compared with the theoretical picture of the basic electronic structure that has been developed for the actinides during the last decade. In particular the experimental data confirm the change from itinerant to localized 5f electron behaviour calculated to take place between plutonium and americium. From experimental data it is shown that the screening of deep core-holes is due to 5f electrons for the lighter actinide elements and 6d electrons for the heavier elements. A simplified model for the full LMTO electronic structure calculations is introduced. In this model the spd and 5f electronic contributions are treated as separable entities. It is shown that the model reproduces quite well the results from the full treatment. The equilibrium volume, cohesive energy and bulk modulus are calculated and compared with experiment. Also the 5f delocalization transition under pressure in Am is treated.

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Organisations: Risø National Laboratory for Sustainable Energy
Authors: Johansson, B. (Ekstern), Skriver, H. L. (Intern)
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Scopus rating (2015): SJR 0.756 SNIP 1.391
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.821 SNIP 1.435
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Scopus rating (2012): SJR 0.929 SNIP 1.302
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BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.068 SNIP 1.285
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.916 SNIP 0.973
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.846 SNIP 0.916
BFI (2008): BFI-level 1
Calculated Structural Phase-Transitions in the Alkaline-Earth Metals

The local-density approximation and the linear muffin-tin orbital method have been used within the atomic-sphere approximation to calculate structural energy differences for all the alkaline earth metals at zero temperature. At ordinary pressure the calculations predict the crystal structure sequence hcp→fcc→bcc as a function of atomic number. As a function of pressure they predict the structure sequence fcc→bcc→hcp. The structural transitions and the onset of superconductivity under pressure are correlated with the d occupation number.

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Authors: Skriver, H. L. (Intern)
Pages: 1768-1772
Publication date: 1982
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Review Letters
Volume: 49
Issue number: 24
ISSN (Print): 0031-9007
Ratings:
BFI (2017): BFI-level 2
BFI (2016): BFI-level 2
Scopus rating (2016): SJR 3.56 SNIP 2.133
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 3.823 SNIP 2.205
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 5.027 SNIP 2.646
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 5.674 SNIP 2.796
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 6.252 SNIP 2.886
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 6.418 SNIP 2.764
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 6.342 SNIP 2.94
DeHaas-van Alphen Effect and LMTO Band-structure of LaSn3

Results of de Haas-van Alphen experiments in the intermetallic compound LaSn3 can be explained by a linear muffin-tin orbital band structure calculation without involving the f bands of lanthanum.
Electronic Structure of the Actinide Metals

General information
State: Published
Organisations: Risø National Laboratory, Risø National Laboratory for Sustainable Energy
Authors: Johansson, B. (Ekstern), Skriver, H. L. (Intern), Krogh Andersen, O. (Ekstern)
Pages: 245-262
Publication date: 1981
Host publication information
Title of host publication: Physics of Solids under High Pressure : Proceedings of an International Symposium
Place of publication: Amsterdam
Publisher: Elsevier Science
Editors: Schilling, J., Shelton, R.
Main Research Area: Technical/natural sciences
Conference: International Symposium on the Physics of Solids under High Pressure, Bad Honnef, 01/01/1981
Source: orbit
Source-ID: 280883
Publication: Research - peer-review › Article in proceedings – Annual report year: 1981

Electronic Transitions in Praseodymium under Pressure

General information
State: Published
Organisations: Risø National Laboratory, Risø National Laboratory for Sustainable Energy
Authors: Skriver, H. L. (Intern)
Pages: 279-282
Publication date: 1981
Host publication information
Title of host publication: Proceedings of the conference Physics of Solids Under High Pressure Using Nuclear Probes'
Place of publication: Amsterdam
Publisher: Elsevier Science
Main Research Area: Technical/natural sciences
Conference: Physics of Solids Under High Pressure Using Nuclear Probes', 01/01/1981
Source: orbit
Source-ID: 281045
Publication: Research › Article in proceedings – Annual report year: 1981

Energy Bands and Mass Enhancement in Yttrium

General information
State: Published
Organisations: Risø National Laboratory, Risø National Laboratory for Sustainable Energy
High Pressure Diffraction Studies of YbH$_2$ up to 28 GPa

**General information**
State: Published
Organisations: Department of Physics, Risø National Laboratory for Sustainable Energy
Authors: Staun Olsen, J. (Ekstern), Buras, B. (Ekstern), Gerward, L. (Intern), Johansson, B. (Ekstern), Lebech, B. (Intern), Skriver, H. L. (Intern), Steenstrup, S. (Ekstern)
Number of pages: 10
Publication date: 1981

**Publication information**
Place of publication: Hamburg
Publisher: Deutsches Elektronen-Synchrotron
Original language: English
Series: DESY SR-81/13
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 281052
Publication: Research › Report – Annual report year: 1981

Shock Anomaly and s-d Transition in High Pressure Lanthanum

**General information**
State: Published
Organisations: Risø National Laboratory, Risø National Laboratory for Sustainable Energy

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**Host publication information**
Title of host publication: Proceedings of the conference Physics of Solids Under High Pressure Using Nuclear Probes
Publisher: Elsevier Science
Editors: Schilling, J., Shelton, R.
Main Research Area: Technical/natural sciences
Conference: Physics of Solids Under High Pressure Using Nuclear Probes, 01/01/1981
Source: orbit
Source-ID: 281051
Publication: Research › Article in proceedings – Annual report year: 1981
The electronic structure of antiferromagnetic chromium

The author has used the local spin density formalism to perform self-consistent calculations of the electronic structure of chromium in the non-magnetic and commensurate antiferromagnetic phases, as a function of the lattice parameter. A change of a few per cent in the atomic radius brings the calculated ground state properties into agreement with experiment. The magnetisation is studied as function of volume in several models, and it is shown that a Stoner picture provides an extremely accurate description of the full calculation provided the sp-d hybridisation is taken into account. It is found that the calculated sublattice magnetisation is extremely sensitive to the exchange-correlation potential used and to the quality of the calculated state density.
The Electronic Structure of Calcium

The electronic structure of calcium under pressure is re-examined by means of self-consistent energy band calculations based on the local density approximation and using the linear muffin-tin orbitals (LMTO) method with corrections to the atomic sphere approximation included. At zero pressure the topology of the Fermi surface as well as the calculated extremal areas are found to depend strongly on the positions of the p and d bands. The positions of the centres of the p and d bands are used as adjustable parameters in order to fit the measured Fermi surface. It is found that shifts of +0.037 and +0.149 Ryd, respectively, relative to the s band, give the best possible agreement. Under increasing pressure the s and p electrons are found to transfer into the d band, and Ca undergoes metal-semimetal-metal electronic transitions. Calculations of the bandstructure and the electronic pressure, including the adjustment to the zero-pressure Fermi surface, allow a simultaneous fit of the measured equation of state and the high-pressure resistivity data to be made.

General information

State: Published
Organisations: Risø National Laboratory, Risø National Laboratory for Sustainable Energy
Authors: Jan, J. (Ekstern), Skriver, H. L. (Intern)
Pages: 805-820
Publication date: 1981
Main Research Area: Technical/natural sciences

Publication information

Journal: Journal of Physics: Condensed Matter
Volume: 11
Issue number: 4
ISSN (Print): 0953-8984
Ratings:
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.881 SNIP 0.754
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.824 SNIP 0.754
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.217 SNIP 0.951
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.297 SNIP 1.022
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.659 SNIP 1.166
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.627 SNIP 1.166
The s-d Transition in Compressed Lanthanum

Calculations of the pressure-volume isotherms for FCC La have been carried out up to pressures of 2 Mbars and temperatures up to 3.4 eV, using the self-consistent linear-muffin-tin-orbital method. The isothermal bulk modulus shows an anomalous stiffening over the pressure range 320-560 kbars, due to termination of the 6s to 5d electronic transition. The effect is calculated to be most pronounced at zero temperature and is largely washed out by a temperature of 3.4 eV. These results lead to a temperature-dependent peak in the lattice Gruneisen parameter, based on a simple Slater-model analysis. Hugoniot calculations using this Gruneisen parameter are in good agreement with experiment and reproduce the anomalous stiffening observed in the shock compression data for La. While the authors also find both significant overlap of the rare-gas cores and melting to occur in the vicinity of the shock anomaly, the present calculations identify the principal cause of the anomaly observed in the La shock data to be the termination of the 6s-5d electronic transition in this material.
5f-Electron Delocalization in Americium

The pressure-volume relation for americium has been obtained without adjustable parameters from self-consistent, spin-polarized band calculations. Around 100 kbar we find a first-order transition to a state with low volume and no spin. This is consistent with preliminary high-pressure measurements.

General information
State: Published
Organisations: Risø National Laboratory, Rise National Laboratory for Sustainable Energy
Authors: Skriver, H. L. (Intern), Andersen, O. K. (Ekstern), Johansson, B. (Ekstern)
Pages: 1230-1233
Publication date: 1980
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Review Letters
Volume: 44
Issue number: 18
ISSN (Print): 0031-9007
Ratings:
BFI (2017): BFI-level 2
BFI (2016): BFI-level 2
Scopus rating (2016): SJR 3.56 SNIP 2.133
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 3.823 SNIP 2.205
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 5.027 SNIP 2.646
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 5.674 SNIP 2.796
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 6.252 SNIP 2.886
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 6.418 SNIP 2.764
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 6.342 SNIP 2.94
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 6.223 SNIP 2.854
Scopus rating (2007): SJR 6.14 SNIP 2.862
Scopus rating (2006): SJR 5.645 SNIP 2.807
Scopus rating (2005): SJR 5.35 SNIP 2.938
Scopus rating (2004): SJR 5.312 SNIP 2.976
Scopus rating (2003): SJR 5.33 SNIP 2.93
Scopus rating (2002): SJR 5.441 SNIP 3.089
Bandstructure and Cohesion of the Actinide Metals

General information
State: Published
Organisations: Risø National Laboratory, Risø National Laboratory for Sustainable Energy
Authors: Andersen, O. K. (Ekstern), Johansson, B. (Ekstern), Skriver, H. L. (Intern)
Pages: 103
Publication date: 1980
Main Research Area: Technical/natural sciences

Publication information
Journal: Physica B: Condensed Matter
Volume: 102
Issue number: 1-3
ISSN (Print): 0921-4526
Ratings:
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.455 SNIP 0.848
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.488 SNIP 0.849
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.553 SNIP 0.942
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.555 SNIP 0.998
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.583 SNIP 0.888
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.586 SNIP 0.809
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.582 SNIP 0.707
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.594 SNIP 0.707
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.582 SNIP 0.646
Scopus rating (2007): SJR 0.551 SNIP 0.619
Scopus rating (2006): SJR 0.541 SNIP 0.617
Scopus rating (2005): SJR 0.589 SNIP 0.547
Scopus rating (2004): SJR 0.661 SNIP 0.625
Scopus rating (2003): SJR 0.541 SNIP 0.481
Scopus rating (2002): SJR 0.516 SNIP 0.52
Scopus rating (2001): SJR 0.605 SNIP 0.46
Scopus rating (2000): SJR 0.658 SNIP 0.578
Scopus rating (1999): SJR 0.658 SNIP 0.509
Calculated Specific Volumes and Magnetic Moments of the 3d Transition Metal Monoxides

We have performed self-consistent, spin-polarized band structure calculations as a function of the lattice spacing for the 3d metal monoxides in order to obtain the equilibrium lattice constants. The calculated binding from the 3d electrons and the occurrence of antiferromagnetism account quantitatively for the experimentally observed trends.

General information
State: Published
Organisations: Risø National Laboratory, Risø National Laboratory for Sustainable Energy
Authors: Skriver, H. L. (Intern), Andersen, O. K. (Ekstern), Johansson, B. (Ekstern)
Pages: 861-862
Publication date: 1980
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Magnetism and Magnetic Materials
Volume: 15-18
Issue number: 1
ISSN (Print): 0304-8853
Ratings:
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.71 SNIP 1.22
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.756 SNIP 1.391
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.821 SNIP 1.435
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.807 SNIP 1.4
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.929 SNIP 1.302
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.068 SNIP 1.285
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.916 SNIP 0.973
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.846 SNIP 0.916
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.861 SNIP 0.897
Scopus rating (2007): SJR 0.708 SNIP 0.848
Scopus rating (2006): SJR 0.832 SNIP 0.877
Scopus rating (2005): SJR 0.683 SNIP 0.693
Scopus rating (2004): SJR 0.792 SNIP 1.037
Scopus rating (2003): SJR 0.975 SNIP 0.897
Scopus rating (2002): SJR 1.188 SNIP 1.079
Scopus rating (2001): SJR 1.139 SNIP 0.952
Scopus rating (2000): SJR 1.19 SNIP 0.935
Scopus rating (1999): SJR 0.904 SNIP 0.885
De Haas-van Alphen Effect and LMTO Bandstructure of NiSi

General information
State: Published
Organisations: Risø National Laboratory, Risø National Laboratory for Sustainable Energy
Authors: Boulet, R. M. (Ekstern), Dunsworth, A. E. (Ekstern), Jan, J. P. (Ekstern), Skriver, H. L. (Intern)
Pages: 2197-2206
Publication date: 1980
Main Research Area: Technical/natural sciences

Publication Information
Journal: Journal of Physics F: Metal Physics
Volume: 10
Issue number: 10
Original language: English
DOIs:
10.1088/0305-4608/10/10/016
Source: orbit
Source-ID: 280892
Publication: Research › Journal article – Annual report year: 1980

Electronic States in Thorium under Pressure
We have used the local-density formalism and the atomic-sphere approximation to calculate self-consistently the electronic properties of thorium at pressures up to 400 kbar. The derived equation of state agrees very well with static pressure experiments and shock data. Below the Fermi level (EF) the electronic band structure is formed by 7s and 6d states while the bottom of a relatively broad 5f band is positioned 0.07 Ry above EF. The calculated extremal areas of the Fermi surface and their calculated pressure dependence agree with earlier calculations and with de Haas-van Alphen measurements supporting the validity of the itinerant description of the 5f electrons for the light actinides. The calculation shows that the gradual s to d transition taking place at pressures up to 200 kbar is the cause of the unusual pressure dependence of the Fermi surface seen experimentally.

General information
State: Published
Organisations: Risø National Laboratory, Risø National Laboratory for Sustainable Energy
Authors: Skriver, H. L. (Intern), Jan, J. P. (Ekstern)
Pages: 1489-1496
Publication date: 1980
Main Research Area: Technical/natural sciences

Publication Information
Journal: Physical Review B Condensed Matter
Volume: 21
Issue number: 4
ISSN (Print): 0163-1829
Ratings:
BFI (2017): BFI-level 1
BFI (2016): BFI-level 2
BFI (2015): BFI-level 2
BFI (2014): BFI-level 2
BFI (2013): BFI-level 2
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 2
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 2
ISI indexed (2011): ISI indexed no
Electronic Structure of Transition Metal Compounds: Ground State Properties of the 3d-Monoxides in the Atomic Sphere Approximation

General information
State: Published
Organisations: Risø National Laboratory, Risø National Laboratory for Sustainable Energy
Authors: Andersen, O. (Ekstern), Skriver, H. L. (Intern), Nohl, H. (Ekstern), Johansson, B. (Ekstern)
Pages: 93-118
Publication date: 1980
Main Research Area: Technical/natural sciences

Publication information
Journal: Pure and Applied Chemistry
Volume: 52
ISSN (Print): 0033-4545
Ratings:
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.972 SNIP 1.049
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.885 SNIP 0.853
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.066 SNIP 1.244
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.134 SNIP 1.145
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.347 SNIP 1.224
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.215 SNIP 1.058
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.987 SNIP 0.882
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.185 SNIP 0.988
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.103 SNIP 1.086
Scopus rating (2007): SJR 1.266 SNIP 1.059
Scopus rating (2006): SJR 0.722 SNIP 0.943
Scopus rating (2005): SJR 0.778 SNIP 0.995
Scopus rating (2004): SJR 0.595 SNIP 0.834
Scopus rating (2003): SJR 0.815 SNIP 0.986
Scopus rating (2002): SJR 0.909 SNIP 0.828
Scopus rating (2001): SJR 0.452 SNIP 0.683
Scopus rating (2000): SJR 0.713 SNIP 0.532
Scopus rating (1999): SJR 0.795 SNIP 0.752
Prediction of Fermi-Surface Pressure Dependence in Rb and Cs

The linear muffin-tin orbitals method of band-structure calculation, combined with a Gaussian integration technique using special directions in the Brillouin zone, has been used to calculate Fermi radii and extremal cross-sectional areas of the Fermi surface in rubidium and cesium. Band shifts were used to achieve optimum agreement with experimental results. Volume derivatives were then obtained by varying the lattice parameter with the band shifts held constant. The significance of this procedure has been discussed in the light of recent theoretical work. The results obtained for the Fermi-surface pressure dependence agree with the limited experimental data available.
Presence and Character of the 5f Electrons in the Actinide Metals
The sensitivity of the Image level binding energy to the occupation of the 5f orbital is pointed out and used to demonstrate the presence of 5f electrons in the uranium metal. It is suggested that the valence band spectrum of uranium might contain satellites originating from excitations to localized 5f-electron configurations. Different kinds of core-hole screenings are discussed for the actinide metals as well as the difference between inner and outer core electron ionizations. Finally, the question of itinerant versus localized 5f behaviour is treated by means of a total energy comparison and the critical separation is found to take place between plutonium and americium.
Band Structure and Optical Properties of Ordered AuCu3
The optical spectra of ordered AuCu3 have been measured at low temperatures by a direct ellipsometric technique. We find several structural elements above the absorption edge as well as in the infrared. The measured spectra are interpreted in terms of the interband absorption calculated from an ab initio band structure obtained by the relativistic linear muffin-tin orbitals method. The band calculation reveals that ordered AuCu3 has distinct copper and gold d bands positioned in and hybridizing with an s band common to copper and gold. The calculated state density is found to be in good agreement with experiment. The Fermi surface is presented and is found to originate mainly in copper 4s and 4p states.

de Haas-van Alphen Effect and LMTO Bandstructure of Al2Cu
The de Haas-van Alphen effect has been measured in the intermetallic compound Al2Cu, and the band structure has been calculated by the LMTO method. The theory provides a reasonable explanation of some low frequencies, and gives excellent agreement with one major larger-frequency branch, but fails to account for other major branches.
de Haas-van Alphen Effect, LMTO Bandstructure and Fermi Surface of beta-AuMg

The de Haas-van Alphen effect has been measured in the ordered alloy beta '-AuMg. The relativistic LMTO bandstructure has been calculated and predicts a Fermi surface in good agreement with experiment. Both bandstructure and Fermi surface are similar in those of other beta brasses with the same number of conduction electrons per unit cell, with the exception of an additional set of electron ellipsoids in an extra conduction band, which owe their existence to the relativistic lowering of the Au 6s band.

Calculated Bulk Properties of the Actinide Metals

Self-consistent relativistic calculations of the electronic properties for seven actinides (Ac-Am) have been performed using the linear muffin-tin orbitals method within the atomic-sphere approximation. Exchange and correlation were included in the local spin-density scheme. The theory explains the variation of the atomic volume and the bulk modulus through the 5f series in terms of an increasing 5f binding up to plutonium followed by a sudden localisation (through complete spin polarisation) in americium.
de Haas-van Alphen Effect, LMTO Bandstructure and Fermi Surface of beta-AgMg

The de Haas-van Alphen effect has been measured in the ordered alloy beta '-AgMg. The relativistic LMTO bandstructure has been calculated, and predicts a Fermi surface in good agreement with experiment. Both bandstructure and Fermi surface are similar to those of other beta brasses with the same number of conduction electrons per unit cell.

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Authors: Dunsworth, A. E. (Ekstern), Jan, J. -. P. (Ekstern), Skriver, H. L. (Intern)
Pages: 1427-1435
Publication date: 1978
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Physics F: Metal Physics
Volume: 8
Issue number: 7
Original language: English
DOIs: 10.1088/0305-4608/8/7/016
Source: orbit
Source-ID: 283314
Effect of Hydrostatic Pressure on Electronic States in Palladium

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Authors: Skriver, H. L. (Intern), Venema, W. (Ekstern), Walker, E. (Ekstern), Griessen, R. (Ekstern)
Pages: 2313-2321
Publication date: 1978
Main Research Area: Technical/natural sciences

Publication information
Journal: JOURNAL OF PHYSICS F-METAL PHYSICS
Volume: 8
Issue number: 11
Original language: English
DOIs: 10.1088/0305-4608/8/11/016
Source: orbit
Source-ID: 283931
Publication: Research - peer-review → Journal article – Annual report year: 1978

Self-Consistent Calculation of Ground-State Properties for Ordered Transition Metal Alloys

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Authors: Skriver, H. L. (Intern), Andersen, O. K. (Ekstern)
Pages: 100-103
Publication date: 1978

Host publication information
Title of host publication: Proceedings of the Transition Metals
Place of publication: Bristol
Publisher: Institute of Physics
Edition: 39
Main Research Area: Technical/natural sciences
Conference: International Conference on Transition Metals, Toronto, Canada, 14/08/1977 - 14/08/1977
Source: orbit
Source-ID: 283933
Publication: Research → Article in proceedings – Annual report year: 1978

Band Structure and Fermi Surface of Cu2Sb by the LMTO Method
The linear muffin-tin orbital (LMTO) method of bandstructure calculation has been applied to the simple tetragonal compound Cu2Sb. The d bands of Cu lie substantially below the Fermi level, and the Fermi surface is a recognizable distortion of the free-electron model. The Fermi surface has sheets in four bands. The first and second bands contain closed sheets, degenerate along a plane in the absence of spin-orbit splitting. The third band contains a multiply-connected sheet. The fourth band consists of undulating columns, degenerate along a plane with the third band in the absence of spin-orbit splitting, and of another closed sheet. Earlier de Haas-van Alphen results are explained semiquantitatively by the model, which also accounts for open orbits seen in high-field magnetoresistance experiments.

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Authors: Jan, J. P. (Ekstern), Skriver, H. L. (Intern)
Pages: 957-967
Publication date: 1977
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Physics F: Metal Physics
Volume: 7
Issue number: 6
Band-Structure of Thallium by the LMTO Method
The relativistic band structure of thallium has been calculated using the linear muffin-tin orbital (LMTO) method. The positions and extents of the bands were found to follow the Wigner-Seitz rule approximately, and the origin of the dispersion of the bands was established from the canonical s and p bands for the HCP structure. Energy bands have been evaluated both with and without spin-orbit coupling which is particularly large in thallium. Energy bands close to the Fermi level were found to be mainly 6p like in character. The 6s states lay below the 6p bands and were separated from them by an energy gap. The 6d and 7s bands were found to be far above the Fermi level and the 5d states were found to be far below it. Fermi surface properties and the electronic specific heat are computed and compared with experiment. The joint density of states has also been computed and is in reasonable agreement with experimental optical properties.

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Authors: Holtham, P. M. (Ekstern), Jan, J. P. (Ekstern), Skriver, H. L. (Intern)
Pages: 635-646
Publication date: 1977
Main Research Area: Technical/natural sciences

Energy Bands and Fermi Surface for beta-MgHg and beta-MgTl
The energy bands of ordered β′-MgHg and β′-MgTl have been calculated by the relativistic linear-muffintin-orbital method. We show how the gross features of the energy bands may be estimated from Wigner-Seitz rules. The densities of states are calculated and the heat capacities derived. The Fermi surfaces are found to be sp-like but there are narrow 5d bands far below—and wide 3d and 6d bands far above—the Fermi levels. For β′-MgHg the calculated angular variation of extremal cross sections of the Fermi surface agrees very well with de Haas-van Alphen data and thereby provide an interpretation of these measurements. The average mass enhancement is found to be 1.6. © 1977 The American Physical Society

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Authors: Skriver, H. L. (Intern)
Pages: 1894-1905
Publication date: 1977
Main Research Area: Technical/natural sciences
Relativistic Band Structure and Fermi Surface of PdTe₂ by the LMTO Method

The energy bands of the trigonal layer compound PdTe₂ have been calculated, using the relativistic linear muffin-tin orbitals method. The bandstructure is separated into three distinct regions with low-lying Te 5s bands, conduction bands formed by Pd 4d and Te 5p states, and high-lying bands formed by Pd 5p, Te 6s and Te 5d states. Density of states and joint density of states have been calculated from the bands determined over the appropriate irreducible zone. The Fermi surface consists of two closed sheets in band 11 and band 13, and sheets in band 12 connected to one another by tubes. The results allow an explanation of most of the de Haas-van Alphen frequencies observed previously.

Band Structure and Fermi-Surface Properties of Ordered beta-Brass

The band structure of ordered β-brass (β′-CuZn) has been calculated throughout the Brillouin zone by the augmented-plane-wave method. The present band model differs from previous calculations with respect to the position and width of the Cu 3d band. The derived dielectric function ε²(ω) and the photoemission spectra agree well with experiments. We find that the main absorption edge as observed in the ε² trace has contributions from conduction-band transitions as well as transitions from the Cu d states. The comparison to photoemission results indicates that the calculated Cu d bands are too narrow, but that their position relative to the Fermi level is correct. The derived Fermi-surface model allows a detailed interpretation of the de Haas-van Alphen (dHvA) data. The present model has no open orbit along for B−∥〈110〉. This agrees with dHvA as well as magnetoresistance measurements. Four new extremal cross sections have been found and related to previously unexplained dHvA frequencies. In general, the Fermi-surface dimensions agree extremely well with dHvA measurements, and the ratios between the experimental and the calculated cyclotron masses vary between 1.18 and 1.43.
Point Measurements of Fermi Velocities by a Time-of-Flight Method

The present paper describes in detail a new method of obtaining information about the Fermi velocity of electrons in metals, point by point, along certain contours on the Fermi surface. It is based on transmission of microwaves through thin metal slabs in the presence of a static magnetic field applied parallel to the surface. The electrons carry the signal across the slab and arrive at the second surface with a phase delay which is measured relative to a reference signal; the velocities are derived by analyzing the magnetic field dependence of the phase delay. For silver we have in this way obtained one component of the velocity along half the circumference of the centrally symmetric orbit for B→∥[100]. The results are in agreement with current models for the Fermi surface. For B→∥[011], the electrons involved are not moving in a symmetry plane of the Fermi surface. In such cases one cannot immediately derive the velocity components, but the method can still be used to provide a comparison of different Fermi surface models. Such a comparison has been made of an augmented-plane-wave model (Christensen) and a Fourier model (Halse), both yielding the experimentally determined areas and cyclotron masses for symmetry orbits of the Fermi surface, but differing slightly at general points. The comparison favors the Fourier model.
Projects:

Phase stability of interstitial austenitic steel
The project is a combined experimental and theoretical approach to establish the basic thermodynamic data for ternary austenitic FeCrNi with a view to improve the stability of steels hardened by insertion of interstitial nitrogen and/or carbon.

Department of Physics
Department of Management Engineering

Center for Nanoteknologi
Period: 01/01/2006 → 31/07/2008
Number of participants: 2
Project ID: 20219
Project participant:
Somers, Marcel A. J. (Intern)
Project Manager, organisational:
Skriver, Hans Lomholt (Intern)

Financing sources
Source: Forskningsrådene - Andre
Name of research programme: Forskningsrådene - Andre
Amount: 2,954,947.00 Danish Kroner

Nanomagnetisme
Department of Physics
Number of participants: 6
Phd Student:
Frandsen, Cathrine (Intern)
Supervisor:
Lefmann, Kim (Ekstern)
Main Supervisor:
Mørup, Steen (Intern)
Examiner:
Skriver, Hans Lomholt (Intern)
McCammon, Catherine (Ekstern)
vander Zaag, Pieter J. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstipendium
Project: PhD

Density functional theory used on biological systems
Department of Physics
Period: 01/02/2000 → 12/02/2004
Number of participants: 6
Phd Student:
Rossmeisl, Jan (Intern)
Supervisor:
Jacobsen, Karsten Wedel (Intern)
Main Supervisor:
Nørskov, Jens Kehlet (Intern)
Examiner:
Skriver, Hans Lomholt (Intern)
Pettersson, Lars G. M. (Ekstern)
Scheffler, Matthias (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

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.

Department of Physics
Aarhus University
Period: 01/09/1998 → 31/12/2005
Number of participants: 12
Project ID: 20018
Project participant:
Jacobsen, Karsten Wedel (Intern)
Skriver, Hans Lomholt (Intern)
Chorkendorff, Ib (Intern)
Schietz, Jakob (Intern)
Horch, Sebastian (Intern)
Nielsen, Jane Hvolbæk (Intern)
Quaade, Ulrich (Intern)
Besenbacher, Flemming (Ekstern)
Stensgaard, Ivan (Ekstern)
Lægsgaard, Erik (Ekstern)
Hammer, Bjørk (Ekstern)

Project Manager, organisational:
Nørskov, Jens Kehlet (Ekstern)

Financing sources
Source: Forsk. Andre statslige danske - Grundforskn.fonden
Name of research programme: Forsk. Andre statslige danske - Grundforskn.fonden
Amount: 28,843,170.00 Danish Kroner

Underseglser af potentielle legeringskatalysatorer ved brug af supersoniske molekylestråler

Department of Physics
Period: 01/02/1998 → 26/09/2001
Number of participants: 5
Phd Student:
Egeberg, Rasmus (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Skriver, Hans Lomholt (Intern)
Besenbacher, Flemming (Intern)
Goodman, Wayne D. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Dislokationens struktur og dynamik

Department of Physics
Period: 01/01/1995 → 25/02/1998
Number of participants: 3
Phd Student:
Rasmussen, Torben (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)
Alloys, multilayers, and interfaces
The goal of the project is to be able to design alloy systems with desirable physical and chemical properties. We also aim at developing theories of alloy formation, heats of solution, and segregation including structural effects. This is achieved through total energy calculations performed within density functional theory. The project involves studies of random as well as partially and completely ordered alloy systems in configurations including multilayers, interfaces, and surfaces. We also study surface alloys. Part of the project involve the development of more accurate but still efficient computational procedures for bulk, surface, and interface systems.

Department of Physics
MPI
Janos Kollár
Uppsala University
Period: 01/09/1993 → …
Number of participants: 5
Project participant:
Ruban, Andrei (Intern)
Andersen, O.K. (Ekstern)
Johansson, Börje (Ekstern)
Vitos, Levente (Ekstern)
Project Manager, organisational:
Skriver, Hans Lomholt (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,000,000.00 Danish Kroner
Project