Excited-state solvation structure of transition metal complexes from molecular dynamics simulations and assessment of partial atomic charge methods

In this work, we investigate the excited-state solute and solvation structure of [Ru(bpy)$_3$]$^{2+}$, [Fe(bpy)$_3$]$^{2+}$, [Fe(bmip)$_2$]$^{2+}$ and [Cu(phen)$_2$]$^{+}$ (bpy = 2,2'-bipyridine; bmip = 2,6-bis(3-methyl-imidazole-1-ylidine)-pyridine; phen = 1,10-phenanthroline) transition metal complexes (TMCs) in terms of solute-solvent radial distribution functions (RDFs) and evaluate the performance of some of the most popular partial atomic charge (PAC) methods for obtaining these RDFs by molecular dynamics (MD) simulations. To this end, we compare classical MD of a frozen solute in water and acetonitrile (ACN) with quantum mechanics/molecular mechanics Born-Oppenheimer molecular dynamics (QM/MM BOMD) simulations. The calculated RDFs show that the choice of a suitable PAC method is dependent on the coordination number of the metal, denticity of the ligands, and type of solvent. It is found that this selection is less sensitive for water than ACN. Furthermore, a careful choice of the PAC method should be considered for TMCs that exhibit a free direct coordination site, such as [Cu(phen)$_2$]$^{+}$. The results of this work show that fast classical MD simulations with ChelpG/RESP or CM5 PACs can produce RDFs close to those obtained by QM/MM MD and thus, provide reliable solvation structures of TMCs to be used, e.g. in the analysis of scattering data.
Theoretical Evidence of Solvent-Mediated Excited-State Dynamics in a Functionalized Iron Sensitizer

The solvent-mediated excited-state dynamics of the COOH-functionalized Fe-carbene photosensitizer $[\text{Fe(bmicp})_2]^{2+}$ (bmicp= 2,6-bis(3-methyl-imidazole-1-ylidine)-4-carboxy-pyridine) is studied by time-dependent density functional theory,
as well as classical and quantum dynamics simulations. We demonstrate the crucial role of the polar acetonitrile solvent in stabilizing the metal-to-ligand charge transfer (MLCT) states of the investigated molecule using the conductor polarizable continuum model. This leads to dynamics that avoid sub-ps back electron transfer to the metal and an exceptionally long-lived 1MLCT state that does not undergo sub-ps 1MLCT → 3MLCT intersystem crossing as it is energetically isolated. We identify two components of the excited-state solvent reorganization process: an initial rotation (∼300 fs) and diffusional dynamics within the local cage surrounding the rotated solvent molecule (∼2 ps). Finally, it is found that the relaxation of the solvent only slightly affects the excited-state population dynamics of [Fe(bmicp)₂]²⁺.

**General information**
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BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
Web of Science (2017): Impact factor 4.484
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195
Web of Science (2016): Impact factor 4.536
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4.68 SJR 1.886 SNIP 1.26
Web of Science (2015): Impact factor 4.509
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 5.08 SJR 2.032 SNIP 1.447
Web of Science (2014): Impact factor 4.772
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 5.14 SJR 2.143 SNIP 1.445
Web of Science (2013): Impact factor 4.835
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 4.98 SJR 2.529 SNIP 1.461
Web of Science (2012): Impact factor 4.814
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 4.92 SJR 2.339 SNIP 1.465
Web of Science (2011): Impact factor 4.805
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Anisotropy enhanced X-ray scattering from solvated transition metal complexes

Time-resolved X-ray scattering patterns from photoexcited molecules in solution are in many cases anisotropic at the ultrafast time scales accessible at X-ray free-electron lasers (XFELs). This anisotropy arises from the interaction of a linearly polarized UV-Vis pump laser pulse with the sample, which induces anisotropic structural changes that can be captured by femtosecond X-ray pulses. In this work, a method for quantitative analysis of the anisotropic scattering signal arising from an ensemble of molecules is described, and it is demonstrated how its use can enhance the structural sensitivity of the time-resolved X-ray scattering experiment. This method is applied on time-resolved X-ray scattering patterns measured upon photoexcitation of a solvated di-platinum complex at an XFEL, and the key parameters involved are explored. It is shown that a combined analysis of the anisotropic and isotropic difference scattering signals in this experiment allows a more precise determination of the main photoinduced structural change in the solute, i.e. the change in Pt-Pt bond length, and yields more information on the excitation channels than the analysis of the isotropic scattering only. Finally, it is discussed how the anisotropic transient response of the solvent can enable the determination of key experimental parameters such as the instrument response function.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Chemistry, Department of Electric Power Engineering, University of Iceland, SLAC National Accelerator Laboratory, Technical University of Denmark
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Issue number: 2
ISSN (Print): 0909-0495
Ratings:
BFI (2019): BFI-level 1
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How to Excite Nuclear Wavepackets into Electronically Degenerate States in Spin-Vibronic Quantum Dynamics Simulations

The excited-state dynamics of two functional Fe-carbene complexes, \([\text{Fe(bmip)}_2]^{2+}\) (bmip = 2,6-bis(3-methyl-imidazole-1-ylidene)-pyridine) and \([\text{Fe(btbip)}_2]^{2+}\) (btbip = 2,6-bis(3-tert-butyl-imidazole-1-ylidene)pyridine), are studied using the spin-vibronic model. In contrast to the usual projection of the ground state nuclear wavefunction onto an excited state surface, the dynamics are initiated by an explicit interaction term between the external time-dependent electric field (laser pulse) and the transition dipole moment of the molecule. The results show that the spin-vibronic model, as constructed directly from electronic structure calculations, exhibits erroneous, polarization-dependent relaxation dynamics stemming from artificial interference of coupled relaxation pathways. This is due to the lack of rotational invariance in the description of excitation into degenerate states. We introduce and discuss a correction using the spherical basis and complex transition dipole moments. This modification in the Hamiltonian leads to rotationally invariant excitation and produces polarization-independent population dynamics.
Perspective: Preservation of coherence in photophysical processes

Coherence is one of the most important phenomena in ultrafast sciences. We give our perspective on the terminology, observation, and preservation of coherence in photophysical processes with some glimpses to the past and some looking-head to what may pave the way for scaling one of the last bastions in ultrafast science, namely, that of mode specific chemistry where it will be possible to break any specific bond by tailoring the pulse, an accomplishment that obviously would be the dream of any chemist.

General information
State: Published
Organisations: Department of Chemistry, King Fahd University of Petroleum and Minerals
Contributors: Sølling, T. I., Møller, K. B.
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Publication information
Journal: Structural Dynamics
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Article number: 060901
ISSN (Print): 2329-7778
Ratings:
Web of Science (2019): Indexed yes
Web of Science (2018): Indexed yes
Scopus rating (2017): CiteScore 3.51 SJR 1.625 SNIP 0.902
Web of Science (2017): Impact factor 3.969
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 2.41 SJR 1.457 SNIP 0.891
Web of Science (2016): Impact factor 2.968
Solution Structure and Ultrafast Vibrational Relaxation of the PtPOP Complex Revealed by ΔSCF-QM/MM Direct Dynamics Simulations

Recent ultrafast experiments have unveiled the time scales of vibrational cooling and decoherence upon photoexcitation of the diplatinum complex [Pt2(P2O5H2)4]4+ in solvents. Here, we contribute to the understanding of the structure and dynamics of the lowest lying singlet excited state of the model photocatalyst by performing potential energy surface calculations and Born–Oppenheimer molecular dynamics simulations in the gas phase and in water. Solvent effects were treated using a multiscale quantum mechanics/molecular mechanics approach. Fast sampling was achieved with a modified version of delta self-consistent field implemented in the grid-based projector-augmented wave density functional theory code. The known structural parameters and the PESs of the first singlet and triplet excited states are correctly reproduced. Besides, the simulations deliver clear evidence that pseudorotation of the ligands in the excited state leads to symmetry lowering of the Pt2P8 core. Coherence decay of Pt–Pt stretching vibrations in solution was found to be governed by vibrational cooling, which is in agreement with previous ultrafast experiments. We also show that the flow of excess Pt–Pt vibrational energy is first directed toward vibrational modes involving the ligands, with the solvent favoring intramolecular vibrational energy redistribution. The results are supported by thorough vibrational analysis in terms of generalized normal modes.

General information
State: Published
Organisations: Department of Chemistry, Technical University of Denmark
Contributors: Levi, G., Pápai, M. I., Henriksen, N. E., Dohn, A. O., Møller, K. B.
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Web of Science (2019): Indexed yes
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
Web of Science (2017): Impact factor 4.484
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195
Web of Science (2016): Impact factor 4.536
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4.68 SJR 1.886 SNIP 1.26
Web of Science (2015): Impact factor 4.509
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 5.08 SJR 2.032 SNIP 1.447
Web of Science (2014): Impact factor 4.772
Grid-Based Projector Augmented Wave (GPAW) Implementation of Quantum Mechanics/Molecular Mechanics (QM/MM) Electrostatic Embedding and Application to a Solvated Dplatinum Complex

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

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Organisations: Department of Chemistry, Department of Physics, Theoretical Atomic-scale Physics, NanoChemistry, University of Iceland, Aalto University
Solvent-Controlled Chemoselectivity in the Photolytic Release of Hydroxamic Acids and Carboxamides from Solid Support

The synthetic utility and theoretical basis of a photolabile hydroxylamine-linker are presented. The developed protocols enable the efficient synthesis and chemoselective photolytic release of either hydroxamates or carboxamides from solid support. The bidetachable mode of the linker unit is uniquely dependent on the solvent. Hydroxamic acids are obtained by performing photolysis in protic solvents, whereas photolysis in aprotic solvents enables the selective release of carboxamides.
Time-resolved X-ray scattering by electronic wave packets: analytic solutions to the hydrogen atom

Modern pulsed X-ray sources permit time-dependent measurements of dynamical changes in atoms and molecules via non-resonant scattering. The planning, analysis, and interpretation of such experiments, however, require a firm and elaborated theoretical framework. This paper provides a detailed description of time-resolved X-ray scattering by non-stationary electronic wave packets in atomic systems. A consistent application of the Waller-Hartree approximation is discussed and different contributions to the total differential scattering signal are identified and interpreted. Moreover, it is demonstrated how the scattering signal of wave packets in the hydrogen atom can be expressed analytically. This permits simulations without numerical integration and establishes a benchmark for both efficiency and accuracy. Based on that, scattering patterns of an exemplary wave packet in the hydrogen atom are computed for different points in time. In doing so, distinct features of time-resolved X-ray scattering by non-stationary electronic wave packets are illustrated and accentuated in greater detail than it has been done before.
Ultrafast X-ray absorption study of longitudinal-transverse phonon coupling in electrolyte aqueous solution

Ultrafast X-ray absorption spectroscopy is applied to study the conversion of longitudinal to transverse phonons in aqueous solution. Permanganate solutes serve as X-ray probe molecules that permit the measurement of the conversion of 13.5 GHz, longitudinal phonons to 27 GHz, transverse phonons that propagate with high-frequency sound speed. The experimental results, combined with QM/MM MD simulations, show that the hydrogen bond network around the charged solutes has a glass-like stiffness that persists for at least tens of picoseconds.

General information
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Organisations: Department of Chemistry, Brown University, Argonne National Laboratory, University of Iceland
Contributors: Jiao, Y., Adams, B. W., Dohn, A. O., Møller, K. B., Jonsson, H., Rose-Petruck, C.
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Journal: Physical Chemistry Chemical Physics
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BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.04 SJR 1.686 SNIP 1.089
Web of Science (2017): Impact factor 3.906
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.06 SJR 1.685 SNIP 1.113
Web of Science (2016): Impact factor 4.123
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.45 SJR 1.725 SNIP 1.205
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.29 SJR 1.771 SNIP 1.239
Web of Science (2014): Impact factor 4.493
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 4.05 SJR 1.72 SNIP 1.207
Web of Science (2013): Impact factor 4.198
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.67 SJR 1.921 SNIP 1.177
Web of Science (2012): Impact factor 3.829
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.6 SJR 1.707 SNIP 1.19
Web of Science (2011): Impact factor 3.573
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.817 SNIP 1.199
Web of Science (2010): Impact factor 3.454
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.147 SNIP 1.364
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.166 SNIP 1.198
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.845 SNIP 1.123
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.477 SNIP 1.118
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.423 SNIP 1.1
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.191 SNIP 1.012
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.146 SNIP 0.929
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.634 SNIP 0.967
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.13 SNIP 1.115
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.948 SNIP 1.079
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.121 SNIP 0
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Ultrafast x-ray scattering studies of solvent and solvation dynamics

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(ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY).
Source: FindIt
Source-ID: 2434457415
Research output: Research - peer-review » Conference abstract in proceedings – Annual report year: 2018

Atomistic characterization of the active-site solvation dynamics of a model photocatalyst

The interactions between the reactive excited state of molecular photocatalysts and surrounding solvent dictate reaction mechanisms and pathways, but are not readily accessible to conventional optical spectroscopic techniques. Here we report an investigation of the structural and solvation dynamics following excitation of a model photocatalytic molecular system \([\text{Ir}_2(\text{dimen})_4]^{2+}\), where dimen is para-diisocyanomenthane. The time-dependent structural changes in this model photocatalyst, as well as the changes in the solvation shell structure, have been measured with ultrafast diffuse X-ray scattering and simulated with Born-Oppenheimer Molecular Dynamics. Both methods provide direct access to the solute-solvent pair distribution function, enabling the solvation dynamics around the catalytically active iridium sites to be robustly characterized. Our results provide evidence for the coordination of the iridium atoms by the acetonitrile solvent and demonstrate the viability of using diffuse X-ray scattering at free-electron laser sources for studying the dynamics of photocatalysis.

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BFI (2019): BFI-level 2
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 12.41 SJR 6.582 SNIP 2.912
Butterfly Deformation Modes in a Photoexcited Pyrazolate-Bridged Pt Complex Measured by Time-Resolved X-Ray Scattering in Solution

Pyrazolate-bridged dinuclear Pt(II) complexes represent a series of molecules with tunable absorption and emission properties that can be directly modulated by structural factors, such as the Pt-Pt distance. However, direct experimental information regarding the structure of the emissive triplet excited state has remained scarce. Using time-resolved wide-angle X-ray scattering (WAXS), the excited triplet state molecular structure of $[\text{Pt}(\text{ppy})(\mu-\text{t-Bu}_{2}\text{pz})]_2$ (ppy = 2-phenylpyridine; t-Bu$_2$pz = 3,5-di-tert-butylpyrazolate), complex 1, was obtained in a dilute (0.5 mM) toluene solution utilizing the monochromatic X-ray pulses at Beamline 11IDD of the Advanced Photon Source. The excited-state structural analysis of 1 was performed based on the results from both transient WAXS measurements and density functional theory calculations to shed light on the primary structural changes in its triplet metal-metal-to-ligand charge-transfer (MMLCT) state, in particular, the Pt-Pt distance and ligand rotation. We found a pronounced Pt-Pt distance contraction accompanied by rotational motions of ppy ligands toward one another in the MMLCT state of 1. Our results suggest that the contraction is larger than what has previously been reported, but they are in good agreement with recent theoretical efforts and suggest the ppy moieties as targets for rational synthesis aimed at tuning the excited-state structure and properties.
Characterizing the Solvated Structure of Photoexcited [Os(terpy)$_2$]$_{2}$ with X-ray Transient Absorption Spectroscopy and DFT Calculations

Characterizing the geometric and electronic structures of individual photoexcited dye molecules in solution is an important step towards understanding the interfacial properties of photo-active electrodes. The broad family of “red sensitizers” based on osmium(II) polypyridyl compounds often undergoes small photo-induced structural changes which are challenging to characterize. In this work, X-ray transient absorption spectroscopy with picosecond temporal resolution is employed to determine the geometric and electronic structures of the photoexcited triplet state of [Os(terpy)$_2$]$^{2+}$ (terpy: 2,2':6',2″-terpyridine) solvated in methanol. From the EXAFS analysis, the structural changes can be characterized by a slight overall expansion of the first coordination shell [OsN$_6$]. DFT calculations supports the XTA results. They also provide additional information about the nature of the molecular orbitals that contribute to the optical spectrum (with TD-DFT) and the near-edge region of the X-ray spectra.

General information
State: Published
Organisations: Department of Chemistry, Tianjin Polytechnic University, Deutsches Elektronen-Synchrotron, Argonne National Laboratory
Contributors: Zhang, X., Pápai, M. I., Møller, K. B., Zhang, J., Canton, S. E.
Number of pages: 9
Publication date: 2016
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Journal: Molecules
Volume: 21
Issue number: 2
ISSN (Print): 1420-3049
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
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Original language: English
Keywords: X-ray transient absorption spectroscopy, Excited-state, Osmium polypyridyl complex
Electronic versions: Characterizing_the_Solvated_Structure_of_Photoexcited.pdf
Effect of tert-Butyl Functionalization on the Photoexcited Decay of a Fe(II)-N-Heterocyclic Carbene Complex

Understanding and subsequently being able to manipulate the excited-state decay pathways of functional transition-metal complexes is of utmost importance in order to solve grand challenges in solar energy conversion and data storage. Herein, we perform quantum chemical calculations and spin-vibronic quantum dynamics simulations on the Fe-N-heterocyclic carbene complex, \([\text{Fe}(\text{btbip})_2]^2+\) (btbip = 2,6-bis(3-tert-butyl-imidazole-1-ylidene)pyridine). The results demonstrate that a relatively minor structural change compared to its parent complex, \([\text{Fe}(\text{bmip})_2]^2+\) (bmip = 2,6-bis(3-methyl-imidazole-1-ylidene)pyridine), completely alters the excited-state relaxation. Ultrafast deactivation of the initially excited metal-to-ligand charge transfer (1,3MLCT) states occurs within 350 fs. In contrast to the widely adopted mechanism of Fe(II) photophysics, these states decay into close-lying singlet metal-centered (1MC) states. This occurs because the tert-butyl functionalization stabilizes the 1MC states, enabling the 1,3MLCT → 1MC population transfer to occur close to the Franck-Condon geometry, making the conversion very efficient. Subsequently, a spin cascade occurs within the MC manifold, leading to the population of triplet and quintet MC states. These results will inspire highly involved ultrafast experiments performed at X-ray free electron lasers and shall pave the way for the design of novel high-efficiency transition-metal-based functional molecules.
Ratings:

BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
Web of Science (2017): Impact factor 4.484
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195
Web of Science (2016): Impact factor 4.536
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4.68 SJR 1.886 SNIP 1.26
Web of Science (2015): Impact factor 4.509
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 5.08 SJR 2.032 SNIP 1.447
Web of Science (2014): Impact factor 4.772
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 5.14 SJR 2.143 SNIP 1.445
Web of Science (2013): Impact factor 4.835
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 4.98 SJR 2.529 SNIP 1.461
Web of Science (2012): Impact factor 4.814
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 4.92 SJR 2.339 SNIP 1.465
Web of Science (2011): Impact factor 4.805
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.462 SNIP 1.362
Web of Science (2010): Impact factor 4.524
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.158 SNIP 1.427
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.883 SNIP 1.04
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Web of Science (2005): Indexed yes
Web of Science (2004): Indexed yes
Web of Science (2003): Indexed yes
Web of Science (2002): Indexed yes
Web of Science (2001): Indexed yes
Electron Transfer and Solvent-Mediated Electronic Localization in Molecular Photocatalysis

This work provides a detailed mechanism for electron transfer in a heterodinuclear complex designed as a model system in which to study homogeneous molecular photocatalysis. With efficient Born–Oppenheimer molecular dynamics simulations, we show how intermediate, charge-separated states can mediate the electron transfer. We observe how Jahn–Teller distortion effects play out in solution, when the molecule has energetically close-lying states, and how this distortion is averaged out in the thermal sampling. Finally, we demonstrate how the solvent helps stabilize and localize the separated charge. The information on the electronic configuration and separate states is of key importance for designing next-generation photocatalysts.

General information
State: Published
Organizations: Department of Chemistry, Department of Physics, Neutrons and X-rays for Materials Physics, University of Hamburg
Contributors: Dohn, A. O., Kjaer, K. S., Harlang, T. B., Canton, S. E., Nielsen, M. M., Møller, K. B.
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BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.7 SJR 1.892 SNIP 1.123
Web of Science (2017): Impact factor 4.7
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.64 SJR 1.804 SNIP 1.199
Web of Science (2016): Impact factor 4.857
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.7 SJR 1.782 SNIP 1.229
Web of Science (2015): Impact factor 4.82
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.69 SJR 1.867 SNIP 1.306
Web of Science (2014): Impact factor 4.762
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 4.9 SJR 1.821 SNIP 1.368
Web of Science (2013): Impact factor 4.794
ISI indexed (2013): ISI indexed yes
Elucidating the Ultrafast Dynamics of Photoinduced Charge Separation in Metalloporphyrin–Fullerene Dyads Across the Electromagnetic Spectrum

Metalloporphyrins are prominent building blocks in the synthetic toolbox of advanced photodriven molecular devices. When the central ion is paramagnetic, the relaxation pathways within the manifold of excited states are highly intricate so that unravelling the intramolecular energy and electron transfer processes is usually a very complex task. This fact is critically hampering the development of applications based on the enhanced coupling offered by the electronic exchange interaction. In this work, the dynamics of charge separation in a copper porphyrin-fullerene are studied with several complementary spectroscopic tools across the electromagnetic spectrum (from near-infrared to X-ray wavelengths), each of them providing specific diagnostics. Correlating the various rates clearly demonstrates that the lifetime of the photoinduced charge-separated state exceeds by about 10-fold that of the isolated photoexcited CuII porphyrin. As
revealed by the spectral modifications in the XANES region, this stabilization is accompanied by a transient change in covalency around the CuII center, which is induced by an enhanced interaction with the C60 moiety. This experimental finding is further confirmed by state-of-the-art calculations using DFT and TD-DFT including dispersion effects that explain the electrostatic and structural origins of this interaction, as the CuII cation becomes ruffled and approaches closer to the fullerene in the charge-separated state. From a methodological point of view, these results exemplify the potential of multielectron excitation features in transient X-ray spectra as future diagnostics of subfemtosecond electronic dynamics. From a practical point of view, this work is paving the way for elucidating out-of-equilibrium electron transfer events coupled to magnetic interaction processes on their intrinsic time-scales.

**General information**
State: Published
Organisations: Department of Chemistry, Tianjin Polytechnic University, Friedrich-Alexander-Universität Erlangen-Nürnberg, Argonne National Laboratory, Uppsala University, Deutsches Elektronen-Synchrotron
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Volume: 120
Issue number: 35
ISSN (Print): 1932-7447
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
Web of Science (2017): Impact factor 4.484
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195
Web of Science (2016): Impact factor 4.536
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4.68 SJR 1.886 SNIP 1.26
Web of Science (2015): Impact factor 4.509
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 5.08 SJR 2.032 SNIP 1.447
Web of Science (2014): Impact factor 4.772
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 5.14 SJR 2.143 SNIP 1.445
Web of Science (2013): Impact factor 4.835
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 4.98 SJR 2.529 SNIP 1.461
Web of Science (2012): Impact factor 4.814
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 4.92 SJR 2.339 SNIP 1.465
Femtosecond X-Ray Scattering Study of Ultrafast Photoinduced Structural Dynamics in Solvated $[\text{Co(terpy)}_2]^{2+}$

We study the structural dynamics of photoexcited $[\text{Co(terpy)}_2]^{2+}$ in an aqueous solution with ultrafast x-ray diffuse scattering experiments conducted at the Linac Coherent Light Source. Through direct comparisons with density functional theory calculations, our analysis shows that the photoexcitation event leads to elongation of the Co-N bonds, followed by coherent Co-N bond length oscillations arising from the impulsive excitation of a vibrational mode dominated by the symmetrical stretch of all six Co-N bonds. This mode has a period of 0.33 ps and decays on a subpicosecond time scale. We find that the equilibrium bond-elongated structure of the high spin state is established on a single-picosecond time scale and that this state has a lifetime of $\sim 7$ ps.

**General information**

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Theoretical Atomic-scale Physics, Department of Chemistry, Lund University
Number of pages: 6
Publication date: 2016
Peer-reviewed: Yes
Observe the solvation dynamics with simultaneous femtosecond X-ray emission spectroscopy and X-ray scattering

In liquid phase chemistry, dynamic solute solvent interactions often govern the path, ultimate outcome, and efficiency of chemical reactions. These steps involve many-body movements on subpicosecond timescales and thus ultrafast structural tools capable of capturing both intramolecular electronic and structural changes, and local solvent structural changes are desired. We have studied the intra- and intermolecular dynamics of a model chromophore, aqueous \( \text{[Fe(bpy)}_3\text{]}^{2+} \), with complementary X-ray tools in a single experiment exploiting intense XFEL radiation as a probe. We monitored the ultrafast structural rearrangement of the solute with X-ray emission spectroscopy, thus establishing time zero for the ensuing X-ray diffuse scattering analysis. The simultaneously recorded X-ray diffuse scattering attenuates reveal slower subpicosecond dynamics triggered by the intramolecular structural dynamics of the photoexcited solute. By simultaneous combination of both methods, we can extract new information about the solvation dynamic processes unfolding during the first picosecond (ps). The measured bulk solvent density increase of 0.2% indicates a dramatic change in the solvation shell around each photoexcited solute, confirming previous ab initio molecular dynamics simulations. Structural changes in the aqueous solvent associated with density and temperature changes occur with similar to 1 ps time constants, characteristic for structural dynamics in water. This slower time scale of the solvent response allows us to directly observe the structure of the excited solute molecules well before the solvent contributions become dominant.

**General information**

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Chemistry, European XFEL, Paul Scherrer Institute, SLAC National Accelerator Laboratory, Hungarian Academy of Sciences, Lund University, European Synchrotron Radiation Facility

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- BFI (2019): BFI-level 1
- Web of Science (2019): Indexed yes
- BFI (2018): BFI-level 1
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 1
- Scopus rating (2017): CiteScore 3.13 SJR 1.331 SNIP 1.015
- Web of Science (2017): Impact factor 3.146
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 3.03 SJR 1.345 SNIP 1.012
- Web of Science (2016): Impact factor 3.177
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): CiteScore 3.25 SJR 1.335 SNIP 1.076
Probing spin-vibronic dynamics using femtosecond X-ray spectroscopy

Ultrafast pump-probe spectroscopy within the X-ray regime is now possible owing to the development of X-ray Free Electrons Lasers (X-FELs) and is opening new opportunities for the direct probing of femtosecond evolution of the nuclei, the electronic and spin degrees of freedom. In this contribution we use wavepacket dynamics of the photoexcited decay of a new Fe(ii) complex, [Fe(bmip)2]^{2+} (bmip = 2,6-bis(3-methyl-imidazole-1-ylidine)pyridine), to simulate the experimental observables associated with femtosecond Fe K-edge X-ray Absorption Near-Edge Structure (XANES) and X-ray emission (XES) spectroscopy. We show how the evolution of the nuclear wavepacket is translated into the spectroscopic signal and the sensitivity of these approaches for following excited state dynamics.
Detailed Characterization of a Nanosecond-Lived Excited State: X-ray and Theoretical Investigation of the Quintet State in Photoexcited [Fe(terpy)(2)](2+)

Theoretical predictions show that depending on the populations of the Fe 3d(xy), 3d(xz), and 3d(yz) orbitals two possible quintet states can exist for the high-spin state of the photoswitchable model system [Fe(terpy)(2)](2+). The differences in the structure and molecular properties of these B-5(2) and E-5 quintets are very small and pose a substantial challenge for experiments to resolve them. Yet for a better understanding of the physics of this system, which can lead to the design of novel molecules with enhanced photoswitching performance, it is vital to determine which high-spin state is reached in the transitions that follow the light excitation. The quintet state can be prepared with a short laser pulse and can be studied with cutting-edge time-resolved X-ray techniques. Here we report on the application of an extended set of X-ray spectroscopy and scattering techniques applied to investigate the quintet state of [Fe(terpy)(2)](2+) 80 ps after light excitation. High-quality X-ray absorption, nonresonant emission, and resonant emission spectra as well as X-ray diffuse scattering data clearly reflect the formation of the high-spin state of the [Fe(terpy)(2)](2+) molecule; moreover, extended X-ray absorption fine structure spectroscopy resolves the Fe-ligand bond-length variations with unprecedented bond-length accuracy in time-resolved experiments. With ab initio calculations we determine why, in contrast to most related systems, one configurational mode is insufficient for the description of the low-spin (LS)-high-spin (HS) transition. We identify the electronic structure origin of the differences between the two possible quintet modes, and finally, we unambiguously identify the formed quintet state as 5E, in agreement with our theoretical expectations.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Risø National Laboratory for Sustainable Energy, Center for Atomic-scale Materials Design, Department of Chemistry, Physical and Biophysical Chemistry, Hungarian Academy of Sciences, Argonne National Laboratory, The Hamburg Centre for Ultrafast Imaging, European XFEL, European Synchrotron Radiation Facility
Pages: 5888-5902
Publication date: 2015
Peer-reviewed: Yes
On the calculation of x-ray scattering signals from pairwise radial distribution functions

We derive a formulation for evaluating (time-resolved) x-ray scattering signals of solvated chemical systems, based on pairwise radial distribution functions, with the aim of this formulation to accompany molecular dynamics simulations. The derivation is described in detail to eliminate any possible ambiguities, and the result includes a modification to the atom-type formulation which to our knowledge is previously unaccounted for. The formulation is numerically implemented and validated.

General information

State: Published
Organisations: Center for Atomic-scale Materials Design, Department of Chemistry, Department of Physics, Neutrons and X-rays for Materials Physics, Physical and Biophysical Chemistry
Contributors: Dohn, A. O., Biasin, E., Haldrup, K., Nielsen, M. M., Henriksen, N. E., Møller, K. B.
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Publication information

Journal: Journal of Physics B: Atomic, Molecular and Optical Physics
Volume: 48
Issue number: 24
Article number: 244010
ISSN (Print): 0953-4075
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 1.77 SJR 0.85 SNIP 0.884
Web of Science (2017): Impact factor 2.119
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 1.22 SJR 0.781 SNIP 0.759
Web of Science (2016): Impact factor 1.792
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 1.19 SJR 1.025 SNIP 1.023
Web of Science (2015): Impact factor 1.833
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 1.5 SJR 1.192 SNIP 0.951
Web of Science (2014): Impact factor 1.975
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 1.62 SJR 1.119 SNIP 0.971
Visualizing the non-equilibrium dynamics of photoinduced intramolecular electron transfer with femtosecond X-ray pulses

Ultrafast photoinduced electron transfer preceding energy equilibration still poses many experimental and conceptual challenges to the optimization of photoconversion since an atomic-scale description has so far been beyond reach. Here we combine femtosecond transient optical absorption spectroscopy with ultrafast X-ray emission spectroscopy and diffuse X-ray scattering at the SACLA facility to track the non-equilibrated electronic and structural dynamics within a bimetallic donor–acceptor complex that contains an optically dark centre. Exploiting the 100-fold increase in temporal resolution as compared with storage ring facilities, these measurements constitute the first X-ray-based visualization of a non-equilibrated intramolecular electron transfer process over large interatomic distances. Experimental and theoretical results establish that mediation through electronically excited molecular states is a key mechanistic feature. The present study demonstrates the extensive potential of femtosecond X-ray techniques as diagnostics of non-adiabatic electron transfer processes in synthetic and biological systems, and some directions for future studies, are outlined.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Center for Atomic-scale Materials Design, Department of Chemistry, Physical and Biophysical Chemistry, Lund University, University of Copenhagen,
Direct Dynamics Studies of a Binuclear Metal Complex in Solution: The Interplay Between Vibrational Relaxation, Coherence, and Solvent Effects

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

General information
State: Published
Organisations: Center for Atomic-scale Materials Design, Department of Chemistry, Physical and Biophysical Chemistry, Department of Physics, NanoChemistry, Neutrons and X-rays for Materials Physics
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Journal: The Journal of Physical Chemistry Letters
Volume: 5
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ISSN (Print): 1948-7185
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 8.37 SJR 4.667 SNIP 1.595
Web of Science (2017): Impact factor 8.709
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.18 SJR 4.602 SNIP 1.651
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 8.04 SJR 4.143 SNIP 1.758
Web of Science (2015): Impact factor 8.539
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 7 SJR 3.725 SNIP 1.71
Web of Science (2014): Impact factor 7.458
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 6.61 SJR 3.529 SNIP 1.608
Web of Science (2013): Impact factor 6.687
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 6.3 SJR 3.965 SNIP 1.742
Web of Science (2012): Impact factor 6.585
ISI indexed (2012): ISI indexed yes
Hexamethylcyclopentadiene: time-resolved photoelectron spectroscopy and ab initio multiple spawning simulations

Progress in our understanding of ultrafast light-induced processes in molecules is best achieved through a close combination of experimental and theoretical approaches. Direct comparison is obtained if theory is able to directly reproduce experimental observables. Here, we present a joint approach comparing time-resolved photoelectron spectroscopy (TRPES) with ab initio multiple spawning (AIMS) simulations on the MS-MR-CASPT2 level of theory. We disentangle the relationship between two phenomena that dominate the immediate molecular response upon light absorption: a spectrally dependent delay of the photoelectron signal and an induction time prior to excited state depopulation in dynamics simulations. As a benchmark molecule, we have chosen hexamethylcyclopentadiene, which shows an unprecedentedly large spectral delay of (310 ± 20) fs in TRPES experiments. For the dynamics simulations, methyl groups were replaced by "hydrogen atoms" having mass 15 and TRPES spectra were calculated. These showed an induction time of (108 ± 10) fs which could directly be assigned to progress along a torsional mode leading to the intersection seam with the molecular ground state. In a stepladder-type approach, the close connection between the two phenomena could be elucidated, allowing for a comparison with other polyenes and supporting the general validity of this finding for their excited state dynamics. Thus, the combination of TRPES and AIMS proves to be a powerful tool for a thorough understanding of ultrafast excited state dynamics in polyenes.
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.04 SJR 1.686 SNIP 1.089
Web of Science (2017): Impact factor 3.906
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.06 SJR 1.685 SNIP 1.113
Web of Science (2016): Impact factor 4.123
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.45 SJR 1.725 SNIP 1.205
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.29 SJR 1.771 SNIP 1.239
Web of Science (2014): Impact factor 4.493
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 4.05 SJR 1.72 SNIP 1.207
Web of Science (2013): Impact factor 4.198
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.67 SJR 1.921 SNIP 1.177
Web of Science (2012): Impact factor 3.829
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.6 SJR 1.707 SNIP 1.19
Web of Science (2011): Impact factor 3.573
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.817 SNIP 1.199
Web of Science (2010): Impact factor 3.454
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.147 SNIP 1.364
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.166 SNIP 1.198
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.845 SNIP 1.123
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.477 SNIP 1.118
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.423 SNIP 1.1
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.191 SNIP 1.012
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.146 SNIP 0.929
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.634 SNIP 0.967
The Non-Ergodic Nature of Internal Conversion

The absorption of light by molecules can induce ultrafast dynamics and coupling of electronic and nuclear vibrational motion. The ultrafast nature in many cases rests on the importance of several potential energy surfaces in guiding the nuclear motion—a concept of central importance in many aspects of chemical reaction dynamics. This Minireview focuses on the non-ergodic nature of internal conversion, that is, on the concept that the nuclear dynamics only sample a reduced phase space, potentially resulting in localization of the dynamics in real space. A series of results that highlight the nonstatistical nature of the excited-state deactivation process is presented. The examples are categorized into four groups. 1) Localization of the energy in one degree of freedom in S2→S1 transitions, in which the transition is either determined by the time spent in the S2→S1 coupling region or by the time it takes to reach it. 2) Localization of energy into a single reactive mode, which is dictated by the internal conversion process. 3) Initiation of the internal conversion by activation of a single complex motion, which then specifically couples to a reactive mode. 4) Nonstatistical internal conversion as a tool to accomplish biomolecular stability. Herein, the discussion on nonstatistical internal conversion in DNA as a mechanism to eliminate Electronic excitation energy is extended to include molecules with an SS bond as a model of the disulfide bridge in peptides. All of these examples are summed up in Kasha’s rule. For systems with multiple degrees of freedom it will be possible to locate an appropriate motion somewhere in phase space that will take the wavepacket to the coupling region and facilitate an ultrafast transition to S1. Once at S1, the momentum of the wavepacket is lost and the only options left are the statistical processes of reaction or light emission.

General information
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Organisations: Department of Chemistry, Maersk Oil Research and Technology Centre, University of Copenhagen
Contributors: Sølling, T. I., Kuhlman, T. S., Stephansen, A. B., Klein, L. B., Møller, K. B.
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.82 SJR 1.28 SNIP 0.781
Web of Science (2017): Impact factor 2.947
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.81 SJR 1.284 SNIP 0.78
Web of Science (2016): Impact factor 3.075
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Time-resolved photoelectron spectroscopy and ab initio multiple spawning studies of hexamethylcyclopentadiene

Time-resolved photoelectron spectroscopy and ab initio multiple spawning were applied to the ultrafast non-adiabatic dynamics of hexamethylcyclopentadiene. The high level of agreement between experiment and theory associates wavepacket motion with a distinct degree of freedom.
Transient Changes in Molecular Geometries and How to Model Them

Light-induced chemical processes are accompanied by molecular motion on the femtosecond time scale. Uncovering this dynamical motion is central to understanding the chemical reaction on a fundamental level. This thesis focuses on the aspects of excess excitation energy dissipation via dynamic changes in molecular structure, vibrations and solvation. In this thesis, we employ our recently developed Quantum-/Molecular -Mechanical Direct Dynamics method to do simulations of transition metal complexes in solution, to uncover their energy dissipation channels, and how they are affected by the solvent. The simulations has also served as benchmarks on this newly developed implementation First, we establish that the chosen model provides a trustworthy description of the systems; since transition metals are heavier than purely organic systems, we test a range of approximations to relativistic quantum mechanic descriptions, to ascertain the accuracy of the quantum model in the Direct Dynamics simulations. We then test - and improve - the framework for calculating the experimental X-ray Diffuse Scattering Difference signal from (any kind of) Molecular Dynamics (MD) simulations. Comparisons of purely classical MD simulations to literature Direct Dynamics simulations delineate the boundaries for the force-field approximation: Classical MD provides a solvent shell response sufficient for experimental fits, but fails to model specific solvent shell changes, such as intercalation. The first Direct Dynamics project of this work focuses on a bi-metallic Ir complex, where the excited state bond formation results in a large Ir-Ir contraction with oscillatory behaviour. Forty simulated excited state trajectories of 3.5 ps each compare well with experimental results, and uncover a new vibrational mode. We observe how the wide distribution of ground state geometries is responsible for decoherence, and that the solvent cage actually facilitates coherent motion, by blocking the newly discovered vibrational mode. We furthermore observe a non-specific, rotational solvent response to the excitation. The second Direct Dynamics project studies the effect of solvation on a bi-centred Ru-Co complex, and we observe how the intercalation solvation response which was lost in the study using only force-fields, is recovered in the Direct Dynamics description.

General information
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Organisations: Center for Atomic-scale Materials Design, Department of Chemistry, Physical and Biophysical Chemistry
Contributors: Dohn, A. O., Møller, K. B., Henriksen, N. E.
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Source: PublicationPreSubmission
Source-ID: 105598969
Research output: Research › Ph.D. thesis – Annual report year: 2015
Filming the Birth of Molecules and Accompanying Solvent Rearrangement

Molecules are often born with high energy and large-amplitude vibrations. In solution, a newly formed molecule cools down by transferring energy to the surrounding solvent molecules. The progression of the molecular and solute-solvent cage structure during this fundamental process has been elusive, and spectroscopic data generally do not provide such structural information. Here, we use picosecond X-ray liquidography (solution scattering) to visualize time-dependent structural changes associated with the vibrational relaxation of I₂ molecules in two different solvents, CCl₄ and cyclohexane. The birth and vibrational relaxation of I₂ molecules and the associated rearrangement of solvent molecules are mapped out in the form of a temporally varying interatomic distance distribution. The I–I distance increases up to ~4 Å and returns to the equilibrium distance (2.67 Å) in the ground state, and the first solvation cage expands by ~1.5 Å along the I–I axis and then shrinks back accompanying the structural change of the I₂ molecule.

General information
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Organisations: X-ray Crystallography, Department of Chemistry, Physical and Biophysical Chemistry, Korean Advanced Institute of Science and Technology (KAIST), European Synchrotron Radiation Facility, Universite Pierre et Marie Curie, Synchrotron Soleil, Inha University
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BFI (2019): BFI-level 2
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BFI (2018): BFI-level 2
Optimizing the Structure of Tetracyanoplatinate (II): A Comparison of Relativistic Density Functional Theory Methods

The geometry of tetracyanoplatinate(II) (TCP) has been optimized with density functional theory (DFT) calculations in order to compare different computational strategies. Two approximate scalar relativistic methods, i.e. the scalar zeroth-order regular approximation (ZORA) and non-relativistic calculations with relativistic effective core potentials (ECPs), were benchmarked against the four-component fully relativistic approach using the Dirac-Coulomb Hamiltonian and all-electron non-relativistic calculations. We find that the 5% contraction of the platinum-carbon bond due to relativistic effects is almost quantitatively reproduced in the ZORA and ECP calculations. In addition, the effect of the exchange-correlation functional and one-electron basis set was studied by employing the two generalized gradient approximation (GGA) functionals, BLYP and PBE, as well as their hybrid version B3LYP and PBE0 in combination with both correlation consistent and Ahlrichs type basis sets. The platinum-carbon bond length (relativistic or non-relativistic) is approximately 1% shorter on using the PBE exchange-correlation functional compared to the BLYP functional but including exact exchange has no significant effect. For the C-N bond these trends are reversed and an order of magnitude smaller. With respect to the basis set dependence we observed that a triple zeta basis set with polarization functions gives in general sufficiently converged results, but while for the Pt-C bond it is advantageous to include extra diffuse functions, this did not turn out to be important for the C-N bond.
Pulling the levers of photophysics

General information
State: Published
Organisations: Department of Chemistry, University of Copenhagen
Contributors: Kuhlman, T. S., Pittelkow, M., Sølling, T. I., Møller, K. B.
Number of pages: 4
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Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 11.31 SJR 6.155 SNIP 2.165
Web of Science (2017): Impact factor 12.102
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 10.8 SJR 5.954 SNIP 2.146
Web of Science (2016): Impact factor 11.994
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 11.13 SJR 5.888 SNIP 2.225
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 10.84 SJR 5.811 SNIP 2.307
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 10.7 SJR 5.702 SNIP 2.198
Web of Science (2013): Impact factor 11.336
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 10.55 SJR 6.407 SNIP 2.329
Web of Science (2012): Impact factor 13.734
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 10.75 SJR 6.063 SNIP 2.361
Web of Science (2011): Impact factor 13.455
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Pulling the Levers of Photophysics: How Structure Controls the Rate of Energy Dissipation

General information
State: Published
Organisations: Physical and Biophysical Chemistry, Department of Chemistry, University of Copenhagen
Contributors: Kuhlman, T. S., Pittelkow, M., Sølling, T. I., Møller, K. B.
Pages: 2303-2306
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Peer-reviewed: Yes

Publication information
Journal: Angewandte Chemie
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Issue number: 8
ISSN (Print): 0044-8249
Ratings:
BFI (2019): BFI-level 1
BFI (2018): BFI-level 1
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BFI (2016): BFI-level 1
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
BFI (2014): BFI-level 1
Web of Science (2014): Indexed yes

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Keywords: Gas-phase reactions, Kinetics, Photophysics, Time-resolved spectroscopy
DOI: 10.1002/anie.201208197
Source: Findit
Source-ID: 2193114239
Research output: Research - peer-review ∙ Journal article – Annual report year: 2013
Quantum-dynamical Modeling of the Rydberg to Valence Excited-State Internal Conversion in Cyclobutanone and Cyclopentanone

In this paper we present 4-state, 5-dimensional Vibronic Coupling Hamiltonians for cyclobutanone and cyclopentanone. Wave packet calculations using these Hamiltonians reveal that for cyclobutanone the (n,3s) to (n,π*) internal conversion involves direct motion in nuclear modes coupling the two states leading to fast population transfer. For cyclopentanone, internal vibrational energy redistribution is a bottleneck for activating reactive nuclear modes leading to slower population transfer.

General information
State: Published
Organisations: Physical and Biophysical Chemistry, Department of Chemistry, University of Copenhagen
Number of pages: 3
Publication date: 2013
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Journal: E P J Web of Conferences
Volume: 41
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Ratings:
Web of Science (2019): Indexed yes
Scopus rating (2017): CiteScore 0.31 SJR 0.194 SNIP 0.233
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 0.28 SJR 0.2 SNIP 0.251
Scopus rating (2015): SJR 0.201 SNIP 0.219
Web of Science (2015): Indexed yes
Scopus rating (2014): SJR 0.19 SNIP 0.165
Scopus rating (2013): SJR 0.166 SNIP 0.126
ISI indexed (2013): ISI indexed no
Scopus rating (2012): SJR 0.177 SNIP 0.163
ISI indexed (2012): ISI indexed no
Scopus rating (2011): SJR 0.155 SNIP 0.201
ISI indexed (2011): ISI indexed no
Toward Highlighting the Ultrafast Electron Transfer Dynamics at the Optically Dark Sites of Photocatalysts

Building a detailed understanding of the structure–function relationship is a crucial step in the optimization of molecular photocatalysts employed in water splitting schemes. The optically dark nature of their active sites usually prevents a complete mapping of the photoinduced dynamics. In this work, transient X-ray absorption spectroscopy highlights the electronic and geometric changes that affect such a center in a bimetallic model complex. Upon selective excitation of the ruthenium chromophore, the cobalt moiety is reduced through intramolecular electron transfer and undergoes a spin flip accompanied by an average bond elongation of 0.20 ± 0.03 Å. The analysis is supported by simulations based on density functional theory structures (B3LYP*/TZVP) and FEFF 9.0 multiple scattering calculations. More generally, these results exemplify the large potential of the technique for tracking elusive intermediates that impart unique functionalities in photochemical devices.

General information
State: Published
Organisations: Department of Physics, Department of Chemistry, Physical and Biophysical Chemistry, Lund University, Argonne National Laboratory, Hungarian Academy of Sciences, European XFEL, SLAC National Accelerator Laboratory, Uppsala University, University of Copenhagen, European Synchrotron Radiation Facility
Pages: 1972-1976
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Peer-reviewed: Yes

Publication information
Journal: The Journal of Physical Chemistry Letters
Volume: 4
Issue number: 11
ISSN (Print): 1948-7185
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 8.37 SJR 4.667 SNIP 1.595
Web of Science (2017): Impact factor 8.709
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.18 SJR 4.602 SNIP 1.651
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 8.04 SJR 4.143 SNIP 1.758
Web of Science (2015): Impact factor 8.539
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Ultrafast Librational Relaxation of H2O in Liquid Water

The ultrafast librational (hindered rotational) relaxation of a rotationally excited H2O molecule in pure liquid water is investigated by means of classical nonequilibrium molecular dynamics simulations and a power and work analysis. This analysis allows the mechanism of the energy transfer from the excited H2O to its water neighbors, which occurs on a sub-100 fs time scale, to be followed in molecular detail, i.e., to determine which water molecules receive the energy and in which degrees of freedom. It is found that the dominant energy flow is to the four hydrogen-bonded water partners in the first hydration shell, dominated by those partners’ rotational motion, in a fairly symmetric fashion over the hydration shell. The minority component of the energy transfer, to these neighboring waters’ translational motion, exhibits an asymmetry in energy reception between hydrogen-bond-donating and -accepting water molecules. The variation of the energy flow characteristics with rotational axis, initial rotational energy excitation magnitude, method of excitation, and temperature is discussed. Finally, the relation of the nonequilibrium results to equilibrium time correlations is investigated.

General information
State: Published
Organisations: Department of Chemistry, Physical and Biophysical Chemistry, Polytechnic University of Catalonia, University of Colorado
Contributors: Petersen, J., Møller, K. B., Rey, R., Hynes, J. T.
Pages: 4541-4552
Between ethylene and polyenes—the non-adiabatic dynamics of cis-dienes.

Using Ab Initio Multiple Spawning (AIMS) with a Multi-State Multi-Reference Perturbation theory (MS-MR-CASPT2) treatment of the electronic structure, we have simulated the non-adiabatic excited state dynamics of cyclopentadiene (CPD) and 1,2,3,4-tetramethyl-cyclopentadiene (Me4-CPD) following excitation to S1. It is observed that torsion around the carbon-carbon double bonds is essential in reaching a conical intersection seam connecting S1 and S0. We identify two timescales; the induction time from excitation to the onset of population transfer back to S0 (CPD: -25 fs, Me4-CPD: -71 fs) and the half-life of the subsequent population transfer (CPD: -28 fs, Me4-CPD: -48 fs). The longer timescales for Me4-CPD are a kinematic consequence of the inertia of the substituents impeding the essential out-of-plane motion that leads to the conical intersection seam. A bifurcation is observed on S1 leading to population transfer being attributable, in a 5 : 2 ratio for CPD and 7 : 2 ratio for Me4-CPD, to two closely related conical intersections. Calculated time-resolved photoelectron spectra are in excellent agreement with experimental spectra validating the simulation results.

General information
State: Published
Organisations: Physical and Biophysical Chemistry, Department of Chemistry, Stanford University
Contributors: Kuhlman, T. S., Glover, W. J., Mori, T., Møller, K. B., Martinez, T. J.
Pages: 193-212
Publication date: 2012
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Ratings:
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.07 SJR 1.524 SNIP 0.903
Web of Science (2017): Impact factor 3.427
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.07 SJR 1.524 SNIP 0.903
Coherent Motion Reveals Non-Ergodic Nature of Internal Conversion between Excited States

We found that specific nuclear motion along low-frequency modes is effective in coupling electronic states and that this motion prevail in some small molecules. Thus, in direct contradiction to what is expected based on the standard models, the internal conversion process can proceed faster for smaller molecules. Specifically, we focus on the S2→S1 internal conversion in cyclobutanone, cyclopentanone, and cyclohexanone. By means of time-resolved mass spectrometry and photoelectron spectroscopy the relative rate of this transition is determined to be 13:2:1. Remarkably, we observe coherent nuclear motion on the S2 surface in a ring-puckering mode and motion along this mode in combination with symmetry considerations allow for a consistent explanation of the observed relative time-scales not afforded by only considering the density of vibrational states or other aspects of the standard models.

General information
State: Published
Organisations: Physical and Biophysical Chemistry, Department of Chemistry, University of Copenhagen
Contributors: Kuhlman, T. S., Sølling, T. I., Møller, K. B.
Pages: 820-827
Publication date: 2012
Peer-reviewed: Yes
Simulating the Ultrafast Excited State Dynamics of Cyclopentadiene and 1,2,3,4-tetramethylcyclopentadiene

**General information**

**State:** Published

**Organisations:** Department of Chemistry, Physical and Biophysical Chemistry, Stanford University

**Contributors:** Kuhlman, T. S., Glover, W. J., Mori, T., Møller, K. B., Martínez, T. J.

**Number of pages:** 1

**Publication date:** 2012

**Peer-reviewed:** No

**Event:** Poster session presented at CECAM conference, Birmingham, United Kingdom.

**Electronic versions:**
- Cyclopentadiene_Birmingham2012.pdf

**Bibliographical note**

Poster for the CECAM conference; High-dimensional Quantum Dynamics: Challenges and Opportunities, Birmingham, April 12-14, 2012

**Source:** dtu

**Source-ID:** u::4036

**Research output:** Research - peer-review › Journal article – Annual report year: 2012

**Symmetry, vibrational energy redistribution and vibronic coupling: The internal conversion processes of cycloketones**

In this paper, we discern two basic mechanisms of internal conversion processes; one direct, where immediate activation of coupling modes leads to fast population transfer and one indirect, where internal vibrational energy redistribution leads to equidistribution of energy, i.e., ergodicity, and slower population transfer follows. Using model vibronic coupling Hamiltonians parameterized on the basis of coupled-cluster calculations, we investigate the nature of the Rydberg to valence excited-state internal conversion in two cycloketones, cyclobutanone and cyclopentanone. The two basic
mechanisms can amply explain the significantly different time scales for this process in the two molecules, a difference which has also been reported in recent experimental findings [T. S. Kuhlman, T. I. Sølling, and K. B. Møller, ChemPhysChem. 13, 820 (2012)]
Time-Resolved X-Ray Diffraction: The Dynamics of the Chemical Bond

We review the basic theoretical formulation for pulsed X-ray scattering on nonstationary molecular states. Relevant time scales are discussed for coherent as well as incoherent X-ray pulses. The general formalism is applied to a nonstationary diatomic molecule in order to highlight the relation between the signal and the time-dependent quantum distribution of internuclear positions. Finally, a few experimental results are briefly discussed.

General information
State: Published
Organisations: Physical Chemistry, Department of Chemistry
Contributors: Møller, K. B., Henriksen, N. E.
Number of pages: 215
Pages: 185-211
Publication date: 2012

Host publication information
Title of host publication: Molecular Electronic Structures of Transition Metal Complexes I
Publisher: Springer
ISBN (Print): 978-3-642-27370-4
Validity of the Bersohn–Zewail model beyond justification

The absorption of probe pulses in ultrafast pump–probe experiments can be determined from the Bersohn–Zewail (BZ) model. The model relies on classical mechanics to describe the dynamics of the nuclei in the excited electronic state prepared by the ultrashort pump pulse. The BZ model provides excellent agreement between the classical trajectory and the average position of the excited state wave packet. By investigating the approximations connecting the nuclear dynamics described by quantum mechanics and the BZ model, we conclude that this agreement goes far beyond the validity of the individual approximations.
Vibrational and Rotational Energy Relaxation in Liquids

Vibrational and rotational energy relaxation in liquids are studied by means of computer simulations. As a precursor for studying vibrational energy relaxation of a solute molecule subsequent to the formation of a chemical bond, the validity of the classical Bersohn-Zewail model for describing the intramolecular dynamics during photodissociation is investigated. The apparent agreement with quantum mechanical calculations is shown to be in contrast to the applicability of the individual approximations used in deriving the model from a quantum mechanical treatment. In the spirit of the Bersohn-Zewail model, the vibrational energy relaxation of I₂ subsequent to photodissociation and recombination in CCl₄ is studied using classical Molecular Dynamics simulations. The vibrational relaxation times and the time-dependent I-I pair distribution function are compared to new experimental results, and a qualitative agreement is found in both cases. Furthermore, the rotational energy relaxation of H₂O in liquid water is studied via simulations and a power-and-work analysis. The mechanism of the energy transfer from the rotationally excited H₂O molecule to its water neighbors is elucidated, i.e. the energy-accepting degrees of freedom of the surrounding solvent water molecules are identified.

General information
State: Published
Organisations: Department of Chemistry, Physical and Biophysical Chemistry
Contributors: Petersen, J., Henriksen, N. E., Møller, K. B.
Number of pages: 86
Publication date: 2012

Publication information
Place of publication: Kgs. Lyngby
Initial Dynamics of The Norrish Type I Reaction in Acetone: Probing Wave Packet Motion

The Norrish Type I reaction in the S1 \((\pi^*\pi)\) state of acetone is a prototype case of ketone photochemistry. On the basis of results from time-resolved mass spectrometry (TRMS) and photoelectron spectroscopy (TRPES) experiments, it was recently suggested that after excitation the wave packet travels toward the S1 minimum in less than 30 fs and stays there for more than 100 picoseconds [Chem. Phys. Lett.2008, 461, 193]. In this work we present simulated TRMS and TRPES signals based on ab initio multiple spawning simulations of the dynamics during the first 200 fs after excitation, getting quite good agreement with the experimental signals. We can explain the ultrafast decay of the experimental signals in the following manner: the wave packet simply travels, mainly along the deplanarization coordinate, out of the detection window of the ionizing probe. This window is so narrow that subsequent revival of the signal due to the coherent deplanarization vibration is not observed, meaning that from the point of view of the experiment the wave packets travels directly to the S1 minimum. This result stresses the importance of pursuing a closer link to the experimental signal when using molecular dynamics simulations in interpreting experimental results.
We present an investigation of structural dynamics in excited-state cations probed in real-time by femtosecond timeresolved ion photofragmentation spectroscopy. From photoelectron spectroscopy data on 1,3-dibromopropane we conclude that the pump pulse ionizes the molecule, populating an excited electronic state of the radical cation. In this state a coherent torsional vibration of the bromomethylene groups with a period of 700 fs is started and probed by photoinduced fragmentation of the molecular cation. The vibrational coherence dephases with the decay of the excited state to the ground state of the cation in 1.6 ps. The real-time probing of the excited-state dynamics is made possible by exploiting the interaction between the two bromine chromophores and its dependence on molecular conformation. This experiment therefore illustrates the applicability of the concept of probing ultrafast molecular dynamics using the intramolecular interaction between two chromophores.
Organisations: Physical Chemistry, Department of Chemistry, Risø National Laboratory for Sustainable Energy, University of Copenhagen
Contributors: Brogaard, R. Y., Møller, K. B., Sølling, T. I.
Pages: 12120-12125
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Peer-reviewed: Yes

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BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.75 SJR 1.17 SNIP 0.964
Web of Science (2017): Impact factor 2.836
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.64 SJR 1.252 SNIP 0.958
Web of Science (2016): Impact factor 2.847
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.78 SJR 1.148 SNIP 1.074
Web of Science (2015): Impact factor 2.883
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.65 SJR 1.159 SNIP 1.069
Web of Science (2014): Impact factor 2.693
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.84 SJR 1.205 SNIP 1.109
Web of Science (2013): Impact factor 2.775
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.78 SJR 1.513 SNIP 1.127
Web of Science (2012): Impact factor 2.771
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.87 SJR 1.422 SNIP 1.131
Web of Science (2011): Impact factor 2.946
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.489 SNIP 1.103
Web of Science (2010): Impact factor 2.732
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.589 SNIP 1.137
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Interpretation of the ultrafast photoinduced processes in pentacene thin films

Ambiguity remains in the models explaining the photoinduced dynamics in pentacene thin films as observed in pump-probe experiments. One model advocates exciton fission as governing the evolution of the initially excited species, whereas the other advocates the formation of an excimeric species subsequent to excitation. On the basis of calculations by a combined quantum mechanics and molecular mechanics (QM/MM) method and general considerations regarding the excited states of pentacene we propose an alternative, where the initially excited species instead undergoes internal conversion to a doubly excited exciton. The conjecture is supported by the observed photophysical properties of pentacene from both static as well as time-resolved experiments.

General information
State: Published
Organisations: Physical Chemistry, Department of Chemistry, University of Southern Denmark, University of Copenhagen
Pages: 3431-3439
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Journal of the American Chemical Society
Volume: 132
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Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 14.05 SJR 8.127 SNIP 2.641
Web of Science (2017): Impact factor 14.357
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 13.18 SJR 7.492 SNIP 2.596
Web of Science (2016): Impact factor 13.858
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 12.81 SJR 6.775 SNIP 2.63
Web of Science (2015): Impact factor 13.038
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 11.92 SJR 6.294 SNIP 2.587
Web of Science (2014): Impact factor 12.113
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 11.38 SJR 5.993 SNIP 2.466
Web of Science (2013): Impact factor 11.444
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 10.37 SJR 6.211 SNIP 2.38
Web of Science (2012): Impact factor 10.677
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 9.94 SJR 5.478 SNIP 2.321
Web of Science (2011): Impact factor 9.907
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 5.167 SNIP 2.138
Web of Science (2010): Impact factor 9.023
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 5.06 SNIP 2.16
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 4.662 SNIP 2.252
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 4.413 SNIP 2.223
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 3.841 SNIP 2.203
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 3.421 SNIP 2.236
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 3.223 SNIP 2.345
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 3.506 SNIP 2.15
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 3.972 SNIP 2.163
On the interpretation of time-resolved anisotropic diffraction patterns

In this paper, we review existing systematic treatments for the interpretation of anisotropic diffraction patterns from partially aligned symmetric top molecules. Such patterns arise in the context of time-resolved diffraction experiments. We calculate diffraction patterns for ground-state NaI excited with an ultraviolet laser. The results are interpreted with the help of a qualitative analytic model, and general recommendations on the analysis and interpretation of anisotropic diffraction patterns are given.
Theory and Simulation of Time-resolved X-ray Diffraction

General information
State: Published
Organisations: Department of Chemistry, Physical Chemistry
Contributors: Møller, K. B.
Publication date: 2010
Peer-reviewed: No
Event: Abstract from Banff Meeting on Structural Dynamics, Banff, Alberta, Canada.
Source: orbit
Theory of time-resolved inelastic x-ray diffraction

Starting from a general theory of time-resolved x-ray scattering, we derive a convenient expression for the diffraction signal based on a careful analysis of the relevant inelastic scattering processes. We demonstrate that the resulting inelastic limit applies to a wider variety of experimental conditions than similar, previously derived formulas, and it directly allows the application of selection rules when interpreting diffraction signals. Furthermore, we present a simple extension to systems simultaneously illuminated by x rays and a laser beam.
Charge-resonance excitations in symmetric molecules - Comparison of linear response DFT with CC3 for the excited states of a model dimer

We present a study on the excited states of an ethylene dimer as to investigate the presence of and perturbation from low-lying charge-resonance states calculated by linear response density functional theory (DFT) using the B3LYP and CAM-B3LYP functionals. The calculations are compared to a reference CC3 calculation revealing a better description of the excited states by CAM-B3LYP than that of B3LYP. The $\Lambda$ parameter introduced by Peach et al. [M.J.G. Peach, P. Benfield, T. Helgaker, D.J. Tozer, J. Chem. Phys. 128 (2008) 044118] does not always reveal the problematic charge-resonance states obtained with B3LYP. The generality of the problem is addressed by taking pentacene as an example.
Comment on "Theoretical Investigation of Perylene Dimers and Excimers and Their Signatures in X-Ray Diffraction"

General information
State: Published
Organisations: Physical Chemistry, Department of Chemistry
Contributors: Kuhlman, T., Lemke, H. T., Sølling, T. I., Velardez, G., Henriksen, N. E., Møller, K. B.
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Peer-reviewed: Yes

Publication information
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Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.75 SJR 1.17 SNIP 0.964
Web of Science (2017): Impact factor 2.836
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.64 SJR 1.252 SNIP 0.958
Web of Science (2016): Impact factor 2.847
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.78 SJR 1.148 SNIP 1.074
Web of Science (2015): Impact factor 2.883
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.65 SJR 1.159 SNIP 1.069
Web of Science (2014): Impact factor 2.693
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.84 SJR 1.205 SNIP 1.109
Web of Science (2013): Impact factor 2.775
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.78 SJR 1.513 SNIP 1.127
Web of Science (2012): Impact factor 2.771
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.87 SJR 1.422 SNIP 1.131
Web of Science (2011): Impact factor 2.946
ISI indexed (2011): ISI indexed yes
Theory and application of time-resolved x-ray diffraction

General information
State: Published
Organisations: Department of Chemistry, Physical Chemistry
Contributors: Møller, K. B.
Number of pages: 60
Publication date: 2009

Host publication information
Title of host publication: Visualizing structures
Place of publication: Lyngby
Source: orbit
Source-ID: 257117
Research output: Research » Conference abstract in proceedings – Annual report year: 2009

New insights on the photodynamics of acetone excited with 270 nm femtosecond pulses

General information
State: Published
Organisations: Physical Chemistry, Department of Chemistry, University of Copenhagen
Contributors: Rusteika, N., Møller, K. B., Sølling, T.
Pages: 193-197
Publication date: 2008
Peer-reviewed: Yes

Publication information
Journal: Chemical Physics Letters
Volume: 461
ISSN (Print): 0009-2614
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.64 SJR 0.656 SNIP 0.61
Web of Science (2017): Impact factor 1.686
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.71 SJR 0.718 SNIP 0.689
Web of Science (2016): Impact factor 1.815
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.83 SJR 0.709 SNIP 0.707
Web of Science (2015): Impact factor 1.86
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.83 SJR 0.755 SNIP 0.765
Web of Science (2014): Impact factor 1.897
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.07 SJR 0.858 SNIP 0.835
Web of Science (2013): Impact factor 1.991
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.2 SJR 1.104 SNIP 0.915
Web of Science (2012): Impact factor 2.145
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.38 SJR 1.159 SNIP 1.004
Web of Science (2011): Impact factor 2.337
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.213 SNIP 0.932
Web of Science (2010): Impact factor 2.282
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.241 SNIP 0.971
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.306 SNIP 0.929
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.437 SNIP 0.994
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.5 SNIP 1.105
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.534 SNIP 1.076
On the theory of time-resolved x-ray diffraction

We derive the basic theoretical formulation for X-ray diffraction with pulsed fields, using a fully quantized description of light and matter. Relevant time scales are discussed for coherent as well as incoherent X-ray pulses, and we provide expressions to be used for calculation of the experimental diffraction signal for both types of X-ray sources. We present a simple analysis of time-resolved X-ray scattering for direct bond breaking in diatomic molecules. This essentially analytical approach highlights the relation between the signal and the time-dependent quantum distribution of internuclear positions, including thermal effects.

General information
State: Published
Organisations: Physical Chemistry, Department of Chemistry
Contributors: Henriksen, N. E., Møller, K. B.
Pages: 558-567
Publication date: 2008
Peer-reviewed: Yes

Publication information
Volume: 112
Issue number: 2
ISSN (Print): 1520-6106
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.13 SJR 1.331 SNIP 1.015
Web of Science (2017): Impact factor 3.146
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.03 SJR 1.345 SNIP 1.012
Web of Science (2016): Impact factor 3.177
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.25 SJR 1.335 SNIP 1.076
Selective bond breakage within the HOD molecule using optimized femtosecond ultraviolet laser pulses

With the HOD molecule initially in its vibrational ground state, we theoretically analyze the laser-induced control of the OD/OH branching ratio D+OH H+OD in the first absorption band. In the weak-field limit, any form of UV-pulse shaping control leads to a branching ratio larger than similar to 2. We obtain in the strong-field limit (peak intensities similar to 10 TW/cm(2)) a branching ratio significantly less than 2. The optimized pulses operate by a pump-dump-pump mechanism, where the dumping to the electronic ground state creates nonstationary vibrational states in HOD.

General information
State: Published
Organisations: Department of Chemistry, Physical Chemistry
Contributors: Tiwari, A. K., Møller, K. B., Henriksen, N. E.
Pages: 065402
Publication date: 2008
Peer-reviewed: Yes

Publication information
Journal: Physical Review A
Volume: 78
Issue number: 6
ISSN (Print): 2469-9926
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.46 SJR 1.288 SNIP 0.886
Web of Science (2017): Impact factor 2.909
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 2.25 SJR 1.482 SNIP 0.985
Web of Science (2016): Impact factor 2.925
Web of Science (2016): Indexed yes
Scopus rating (2015): CiteScore 2.06 SJR 1.747 SNIP 1.008
Web of Science (2015): Impact factor 2.765
Web of Science (2015): Indexed yes
Scopus rating (2014): CiteScore 2.46 SJR 2.201 SNIP 1.163
Web of Science (2014): Indexed yes
Scopus rating (2013): CiteScore 2.86 SJR 2.305 SNIP 1.166
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): CiteScore 2.81 SJR 2.519 SNIP 1.231
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): CiteScore 2.79 SJR 2.316 SNIP 1.252
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 2.4 SNIP 1.211
Web of Science (2010): Indexed yes
Scopus rating (2009): SJR 2.469 SNIP 1.346
Web of Science (2009): Indexed yes
Scopus rating (2008): SJR 2.536 SNIP 1.231
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.524 SNIP 1.203
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.834 SNIP 0.968
Web of Science (2006): Indexed yes
Theoretical investigation of perylene dimers and excimers and their signatures in X-ray diffraction

The structures of the ground and excimer states of perylene pairs are calculated [using density functional theory (DFT) and time-dependent DFT techniques] in a free as well as a crystal environment, and their spectroscopic properties are studied for the most stable configurations. The vertical transition energies for the absorption and emission bands are obtained, and they are in good agreement with experimental data. In these calculations, up to six excited states are considered. With the calculated structures of the ground and excimer states, the scattering factors are analyzed as a function of the concentration of excimers in a crystal. The intensity of the 110, 005, and 0 10 0 reflections are found to be fairly sensitive to the presence of excimers in the crystal. The finite (nanosecond) lifetime of the excimer may make it possible to observe this state using time-resolved X-ray diffraction techniques.

General information
State: Published
Organisations: Physical Chemistry, Department of Chemistry, Norwegian University of Science and Technology, University of Copenhagen
Contributors: Velardez, G., Lemke, H. T., Breiby, D., Nielsen, M. M., Møller, K. B., Henriksen, N. E.
Pages: 8179-8187
Publication date: 2008
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry A
Volume: 112
Issue number: 35
ISSN (Print): 1089-5639
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.75 SJR 1.17 SNIP 0.964
Web of Science (2017): Impact factor 2.836
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.64 SJR 1.252 SNIP 0.958
Web of Science (2016): Impact factor 2.847
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.78 SJR 1.148 SNIP 1.074
Web of Science (2015): Impact factor 2.883
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.65 SJR 1.159 SNIP 1.069
Web of Science (2014): Impact factor 2.693
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.84 SJR 1.205 SNIP 1.109
Web of Science (2013): Impact factor 2.775
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.78 SJR 1.513 SNIP 1.127
Web of Science (2012): Impact factor 2.771
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.87 SJR 1.422 SNIP 1.131
Web of Science (2011): Impact factor 2.946
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.489 SNIP 1.103
Web of Science (2010): Impact factor 2.732
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.589 SNIP 1.137
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.822 SNIP 1.099
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.951 SNIP 1.139
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.774 SNIP 1.204
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.847 SNIP 1.219
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.711 SNIP 1.233
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.843 SNIP 1.256
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.869 SNIP 1.229
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.826 SNIP 1.202
Web of Science (2001): Indexed yes
Wave Packet Simulation of Nonadiabatic Dynamics in Highly Excited 1,3-Dibromopropane

We have conducted wave packet simulations of excited-state dynamics of 1,3-dibromopropane (DBP) with the aim of reproducing the experimental results of the gas-phase pump-probe experiment by Kotting et al. [Kotting, C.; Diau, E. W.-G.; Solling, T. L.; Zewail, A. H. J. Phys. Chem. A 2001106, 7530]. In the experiment, DBP is excited to a Rydberg state 8 eV above the ground state. The interpretation of the results is that a torsional motion of the bromomethylene groups with a vibrational period of 680 is is activated upon excitation. The Rydberg state decays to a valence state, causing a dissociation of one of the carbon bromine bonds on a time scale of 2.5 ps. Building the theoretical framework for the wave packet propagation around this model of the reaction dynamics, the Simulations reproduce, to a good extent, the time scales observed in the experiment. Furthermore, the Simulations provide insight into how the torsion motion influences the bond breakage, and we can conclude that the mechanism that delays the dissociation is solely the electronic transition from the Rydberg state to the valence state and does not involve, for example, intramolecular vibrational energy redistribution (IVR).
Controlling the spreading of wave packets of a dissociating molecule

A first-order perturbation theoretic approach within the electric-dipole approximation is used to study the time evolution of wave packets created by linearly chirped laser pulses on a repulsive potential of Br₂. Our calculations show that negatively chirped pulses focus the wave packet in the Franck-Condon region whereas, as well known, the positively chirped pulses focus the wave packet in the asymptotic region. For the negatively chirped pulses, we show that the time corresponding to the minimum in the width of the wave packet can be predicted by an analytical formula. (C) 2007 Elsevier B.V. All rights reserved.
Kan man filme en kemisk reaktion?

General information
State: Published
Organisations: Physical Chemistry, Department of Chemistry
Contributors: Henriksen, N. E., Møller, K. B., Petersen, J.
Pages: 148-160
Publication date: 2007

Host publication information
Title of host publication: Nye Kemiske Horisonter
Place of publication: Lyngby
Publisher: Technical University of Denmark (DTU)
ISBN (Print): 87-91233-13-5
Electronic versions: kemibog 3105.pdf
Source: orbit
Source-ID: 201604
Research output: Education - peer-review › Book chapter – Annual report year: 2007

Quantum Hydrodynamics And a Moment Approach to Mixed Quantum-Classical Theory

General information
State: Published
Organisations: Physical Chemistry, Department of Chemistry
Contributors: Burghardt, I., Møller, K. B., Hughes, K.
Pages: 375-406
Publication date: 2007

Host publication information
Title of host publication: Quantum Dynamics of Complex Molecular Systems
Publisher: Springer
ISBN (Print): 35-40-34458-6
(Springer Series in Chemical Physics; No. 83).
Source: orbit
Source-ID: 189794
Research output: Research - peer-review › Book chapter – Annual report year: 2007
Dissipative quantum dynamics with trajectories

General information
State: Published
Organisations: Department of Chemistry, Physical Chemistry
Contributors: Møller, K. B., Burghardt, I.
Number of pages: 89
Pages: 80-89
Publication date: 2006

Host publication information
Title of host publication: Dynamics of open quantum systems
Place of publication: Daresbury
Publisher: CCP6
Editor: Hughes, K.
ISBN (Print): 978-0-9545289-6-6
Source: orbit
Source-ID: 197489
Research output: Research › Article in proceedings – Annual report year: 2006

Selective bond breakage in HOD with shaped UV-femtosecond laser pulses

General information
State: Published
Organisations: Department of Chemistry
Contributors: Møller, K. B., Westtoft, H. C., Henriksen, N. E.
Pages: 65-69
Publication date: 2006
Peer-reviewed: Yes

Publication information
Journal: Chemical Physics Letters
Volume: 419
Issue number: 1-3
ISSN (Print): 0009-2614
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.64 SJR 0.656 SNIP 0.61
Web of Science (2017): Impact factor 1.686
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.71 SJR 0.718 SNIP 0.689
Web of Science (2016): Impact factor 1.815
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.83 SJR 0.709 SNIP 0.707
Web of Science (2015): Impact factor 1.86
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.83 SJR 0.755 SNIP 0.765
Web of Science (2014): Impact factor 1.897
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.07 SJR 0.856 SNIP 0.835
Web of Science (2013): Impact factor 1.991
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Isotope effects in the photofragmentation of symmetric molecules: The branching ratio of OD/OH in water

With HOD initially in its vibrational ground state, we present a new detailed interpretation of the OD/OH branching ratio (similar to 3) in the photoinduced process D+OH H+OD, in the first absorption band. Using semiclassical arguments, we show that the branching ratio has little to do with the initial distribution of configurations, but the initial momentum distribution plays a key role in determination of the branching ratio. The formation of D+OH arises from initial situations where OD is stretching, and it stretches faster than OH, whereas all other motions lead to H+OD. This picture is confirmed by quantum wave-packet calculations. (c) 2005 American Institute of Physics.

General information
State: Published
Organisations: Physical Chemistry, Department of Chemistry, Universität Würzburg
Contributors: Henriksen, N. E., Møller, K. B., Engel, V.
Pages: 204320
Publication date: 2005
On the coupling between molecular diffusion and solvation shell exchange

The connection between diffusion and solvent exchanges between first and second solvation shells is studied by means of molecular dynamics simulations and analytic calculations, with detailed illustrations for water exchange for the Li$^+$ and Na$^+$ ions, and for liquid argon. First, two methods are proposed which allow, by means of simulation, to extract the quantitative speed-up in diffusion induced by the exchange events. Second, it is shown by simple kinematic considerations that the instantaneous velocity of the solute conditions to a considerable extent the character of the exchanges. Analytic formulas are derived which quantitatively estimate this effect, and which are of general applicability to molecular diffusion in any thermal fluid. Despite the simplicity of the kinematic considerations, they are shown to well describe many aspects of solvent exchange/diffusion coupling features for nontrivial systems. (c) 2005 American Institute of Physics.
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 2.5 SJR 1.252 SNIP 0.926
Web of Science (2017): Impact factor 2.843
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.13 SJR 1.486 SNIP 0.964
Web of Science (2016): Impact factor 2.965
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 1.98 SJR 1.255 SNIP 0.964
Web of Science (2015): Impact factor 2.894
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.54 SJR 1.446 SNIP 1.02
Web of Science (2014): Impact factor 2.952
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.95 SJR 1.559 SNIP 1.174
Web of Science (2013): Impact factor 3.122
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.86 SJR 1.832 SNIP 1.137
Web of Science (2012): Impact factor 3.164
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.07 SJR 1.845 SNIP 1.215
Web of Science (2011): Impact factor 3.333
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.777 SNIP 1.064
Web of Science (2010): Impact factor 2.921
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.04 SNIP 1.119
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.27 SNIP 1.144
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.245 SNIP 1.13
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.254 SNIP 1.287
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.323 SNIP 1.349
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.272 SNIP 1.39
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.275 SNIP 1.395
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.28 SNIP 1.382
Web of Science (2002): Indexed yes
Theoretical perspectives on ultrafast IR spectroscopy in water

General information
State: Published
Organisations: Department of Chemistry, Polytechnic University of Catalonia, Ecole Normale Superieure
Contributors: Møller, K. B., Rey, R., Hynes, J. T.
Pages: 195-201
Publication date: 2005

Host publication information
Title of host publication: Time Resolved Vibrational Spectroscopy : Proceedings of the XI TRVS International Conference
Place of publication: Florence
Publisher: Leo S. Olschki
Editors: Califano, S., Foggi, P., Righini, R.
ISBN (Print): 88-22-25479-1
Source: orbit
Source-ID: 43073
Research output: Research › Article in proceedings – Annual report year: 2005

Approaches to wave-packet imaging using femtosecond ionization spectroscopy

General information
State: Published
Organisations: Department of Chemistry, Universität Würzburg
Contributors: Gräfe, S., Scheidel, D., Engel, V., Henriksen, N. E., Møller, K. B.
Pages: 8954-8960
Publication date: 2004
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry A
Volume: 108
ISSN (Print): 1089-5639
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.75 SJR 1.17 SNIP 0.964
Web of Science (2017): Impact factor 2.836
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.64 SJR 1.252 SNIP 0.958
Web of Science (2016): Impact factor 2.847
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.78 SJR 1.148 SNIP 1.074
Web of Science (2015): Impact factor 2.883
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.65 SJR 1.159 SNIP 1.069
Web of Science (2014): Impact factor 2.693
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.84 SJR 1.205 SNIP 1.109
Web of Science (2013): Impact factor 2.775
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.78 SJR 1.513 SNIP 1.127
Web of Science (2012): Impact factor 2.771
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.87 SJR 1.422 SNIP 1.131
Web of Science (2011): Impact factor 2.946
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.489 SNIP 1.103
Web of Science (2010): Impact factor 2.732
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.589 SNIP 1.137
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.822 SNIP 1.099
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.951 SNIP 1.139
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.774 SNIP 1.204
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.847 SNIP 1.219
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.711 SNIP 1.233
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.843 SNIP 1.256
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.869 SNIP 1.229
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.826 SNIP 1.202
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.94 SNIP 1.282
Femtokemi: Kemiens afgørende øjeblikke

General information
State: Published
Organisations: Department of Chemistry
Contributors: Henriksen, N. E., Møller, K. B., Sølling, T. I.
Pages: 15-17
Publication date: 2004
Peer-reviewed: Unknown

Publication information
Journal: Dansk Kemi
Volume: 85
Issue number: 8
ISSN (Print): 0011-6335
Ratings:
ISI indexed (2013): ISI indexed no
ISI indexed (2012): ISI indexed no
ISI indexed (2011): ISI indexed no
Web of Science (2007): Indexed yes
Web of Science (2004): Indexed yes
Original language: Danish
Source: orbit
Source-ID: 43203
Research output: Communication – Journal article – Annual report year: 2004

Hydrogen bond dynamics and ultrafast IR spectroscopy of water: a theoretical study

General information
State: Published
Organisations: Department of Chemistry, Polytechnic University of Catalonia, Ecole Normale Superieure
Contributors: Møller, K. B., Rey, R., Hynes, J. T.
Pages: 1275-1289
Publication date: 2004
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry A
Volume: 108
ISSN (Print): 1089-5639
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.75 SJR 1.17 SNIP 0.964
Web of Science (2017): Impact factor 2.836
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.64 SJR 1.252 SNIP 0.958
Web of Science (2016): Impact factor 2.847
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.78 SJR 1.148 SNIP 1.074
Web of Science (2015): Impact factor 2.883
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.65 SJR 1.159 SNIP 1.069
Web of Science (2014): Impact factor 2.693
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.84 SJR 1.205 SNIP 1.109
Web of Science (2013): Impact factor 2.775
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.78 SJR 1.513 SNIP 1.127
Web of Science (2012): Impact factor 2.771
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.87 SJR 1.422 SNIP 1.131
Web of Science (2011): Impact factor 2.946
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.489 SNIP 1.103
Web of Science (2010): Impact factor 2.732
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.589 SNIP 1.137
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.822 SNIP 1.099
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.951 SNIP 1.139
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.774 SNIP 1.204
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.847 SNIP 1.219
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.711 SNIP 1.233
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.843 SNIP 1.256
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.869 SNIP 1.229
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.826 SNIP 1.202
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.94 SNIP 1.282
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.443 SNIP 1.6
Original language: English
On ultrafast IR spectroscopy in water

General information
State: Published
Organisations: Department of Chemistry, Polytechnic University of Catalonia, Ecole Normale Superieure
Contributors: Møller, K. B., Rey, R., Hynes, J. T.
Pages: 177-180
Publication date: 2004

Host publication information
Title of host publication: Femtochemistry and Femtobiology: Ultrafast Events in Molecular Science
Place of publication: Amsterdam
Publisher: Elsevier
Editors: Martin, M. M., Hynes, J. T.
ISBN (Print): 0-444-51656-5
Source: orbit
Source-ID: 181658
Research output: Research - peer-review › Article in proceedings – Annual report year: 2004

Quantum control fields from instantaneous dynamics

General information
State: Published
Organisations: Department of Chemistry, Universität Würzburg
Contributors: Gräfe, S., Marquetand, P., Engel, V., Henriksen, N. E., Møller, K. B.
Pages: 180-185
Publication date: 2004
Peer-reviewed: Yes

Publication information
Journal: Chemical Physics Letters
Volume: 398
ISSN (Print): 0009-2614
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.64 SJR 0.656 SNIP 0.61
Web of Science (2017): Impact factor 1.686
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.71 SJR 0.718 SNIP 0.689
Web of Science (2016): Impact factor 1.815
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.83 SJR 0.709 SNIP 0.707
Web of Science (2015): Impact factor 1.86
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.83 SJR 0.755 SNIP 0.765
Web of Science (2014): Impact factor 1.897
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.07 SJR 0.858 SNIP 0.835
Web of Science (2013): Impact factor 1.991
ISI indexed (2013): ISI indexed yes
Quantum hydrodynamics: Non-equilibrium and mixed quantum-classical systems

General information
State: Published
Organisations: Department of Chemistry, Ecole Normale Superieure, Universite de Montpellier
Contributors: Møller, K. B., Burghardt, I., Parlant, G.
Publication date: 2004
Peer-reviewed: No
Event: Poster session presented at Sanibel Symposium, .
Source: orbit
Source-ID: 59671
Research output: Research - poster-review → Poster – Annual report year: 2004
Supressing the spreading of continuum wave packets via chirped laser pulses

**General information**

State: Published  
Organisations: Department of Chemistry, University of Florida  
Contributors: Manescu, C., Krause, J. L., Møller, K. B., Henriksen, N. E.  
Pages: 8840-8847  
Publication date: 2004  
Peer-reviewed: Yes

**Publication information**

Journal: Journal of Physical Chemistry A  
Volume: 108  
ISSN (Print): 1089-5639  
Ratings:  
BFI (2019): BFI-level 1  
Web of Science (2019): Indexed yes  
BFI (2018): BFI-level 1  
Web of Science (2018): Indexed yes  
BFI (2017): BFI-level 1  
Scopus rating (2017): CiteScore 2.75 SJR 1.17 SNIP 0.964  
Web of Science (2017): Impact factor 2.836  
Web of Science (2017): Indexed yes  
BFI (2016): BFI-level 1  
Scopus rating (2016): CiteScore 2.64 SJR 1.252 SNIP 0.958  
Web of Science (2016): Impact factor 2.847  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 1  
Scopus rating (2015): CiteScore 2.78 SJR 1.148 SNIP 1.074  
Web of Science (2015): Impact factor 2.883  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 1  
Scopus rating (2014): CiteScore 2.65 SJR 1.159 SNIP 1.069  
Web of Science (2014): Impact factor 2.693  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 1  
Scopus rating (2013): CiteScore 2.84 SJR 1.205 SNIP 1.109  
Web of Science (2013): Impact factor 2.775  
ISI indexed (2013): ISI indexed yes
Ultrafast non-Franck-Condon transitions: is it possible?

General information
State: Published
Organisations: Department of Chemistry
Contributors: Henriksen, N. E., Møller, K. B.
Pages: 135-138
Publication date: 2004
Ultrafast non-Franck-Condon transitions via a two-pulse scheme

General information
State: Published
Organisations: Department of Chemistry
Contributors: Møller, K. B., Henriksen, N. E.
Pages: 134-139
Publication date: 2004
Peer-reviewed: Yes

Publication information
Journal: Chemical Physics Letters
Volume: 385
ISSN (Print): 0009-2614
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.64 SJR 0.656 SNIP 0.61
Web of Science (2017): Impact factor 1.686
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.71 SJR 0.718 SNIP 0.689
Web of Science (2016): Impact factor 1.815
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.83 SJR 0.709 SNIP 0.707
Web of Science (2015): Impact factor 1.86
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.83 SJR 0.755 SNIP 0.765
Web of Science (2014): Impact factor 1.897
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.07 SJR 0.858 SNIP 0.835
Web of Science (2013): Impact factor 1.991
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.2 SJR 1.104 SNIP 0.915
Web of Science (2012): Impact factor 2.145
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.38 SJR 1.159 SNIP 1.004
Web of Science (2011): Impact factor 2.337
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.213 SNIP 0.932
Web of Science (2010): Impact factor 2.282
Ultrafast vibrational population dynamics of water and related systems: A theoretical perspective

General information
State: Published
Organisations: Department of Chemistry, Polytechnic University of Catalonia, Ecole Normale Superieure
Contributors: Rey, R., Møller, K. B., Hynes, J. T.
Pages: 1915-1928
Publication date: 2004
Peer-reviewed: Yes

Publication information
Journal: Chemical Reviews
Volume: 104
ISSN (Print): 0009-2665
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 51.08 SJR 23.414 SNIP 11.97
Web of Science (2017): Impact factor 52.613
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 42.79 SJR 19.51 SNIP 10.358
Web of Science (2016): Impact factor 47.928
Web of Science (2016): Indexed yes
Femtosecond IR spectroscopy of water: a theoretical study

General information
State: Published
Organisations: Department of Chemistry, Polytechnic University of Catalonia, Ecole Normale Superieure
Contributors: Möller, K. B., Rey, R., Hynes, J. T.
Publication date: 2003
Peer-reviewed: Yes
**Femtosecond IR spectroscopy of water: a theoretical study**

**General information**
State: Published
Organisations: Department of Chemistry, Polytechnic University of Catalonia, Ecole Normale Superieure
Contributors: Møller, K. B., Rey, R., Hynes, J. T.
Publication date: 2003
Peer-reviewed: No
Source: orbit
Source-ID: 36019
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2003

**Instantaneous non-vertical electronic transitions with shaped femtosecond laser pulses: Is it possible?**

**General information**
State: Published
Organisations: Department of Chemistry
Contributors: Henriksen, N. E., Møller, K. B.
Publication date: 2003
Peer-reviewed: No
Source: orbit
Source-ID: 36116
Research output: Research › Poster – Annual report year: 2003

**Instantaneous non-vertical electronic transitions with shaped femtosecond laser pulses: Is it possible?**

**General information**
State: Published
Organisations: Department of Chemistry
Contributors: Henriksen, N. E., Møller, K. B.
Publication date: 2003
Peer-reviewed: Yes
Source: orbit
Source-ID: 36115
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2003

In molecular electronic transitions, a vertical transition can be induced by an ultrashort laser pulse. That is, a replica of the initial nuclear state-times the transition dipole moment of the electronic transition-can be created instantaneously (on the time scale of nuclear motion) in the excited electronic state. Now, applying pulse shaping via the modulation of the phases of each spectral component of an ultrashort pulse, it is tempting to ask whether it is also possible to induce instantaneous nonvertical transitions to bound electronic states, provided that the phases of each spectral component of the pulse are set to appropriate values at the discrete frequencies corresponding to the energy levels of the potential. We analyze the problem in the weak-field limit, and show that such a phase requirement cannot be encoded into an ultrashort pulse. This result is equivalent to the statement that it is not possible to move matter faster than the time associated with the natural (field-free) dynamics of the system.
Ultrafast IR spectroscopy of water: a theoretical study

General information
State: Published
Organisations: Department of Chemistry, Polytechnic University of Catalonia, Ecole Normale Superieure
Contributors: Møller, K. B., Rey, R., Hynes, J. T.
Publication date: 2003
Peer-reviewed: No
Event: Poster session presented at 11th International Conference on Time-Resolved Vibrational Spectroscopy, Castiglione delle Pescaia, Italy.
Source: orbit
Source-ID: 36017
Research output: Research › Poster – Annual report year: 2003

Ultrafast IR spectroscopy of water: a theoretical study

General information
State: Published
Organisations: Department of Chemistry, Polytechnic University of Catalonia, Ecole Normale Superieure
Contributors: Møller, K. B., Rey, R., Hynes, J. T.
Publication date: 2003
Peer-reviewed: No
Event: Abstract from 11th International Conference on Time-Resolved Vibrational Spectroscopy, Castiglione delle Pescaia, Italy.
Source: orbit
Source-ID: 36018
Research output: Research › Conference abstract for conference – Annual report year: 2003

Hydrogen bond dynamics and ultrafast IR spectroscopy of water

General information
Kinetics modeling of dynamics: the case of femtosecond-activated direct reactions
A comparison between a kinetics model and the familiar picture of femtosecond dynamics for direct bond breakage is presented. The kinetics model involves a series of consecutive first-order reactions between transient configurations of the molecule as the bond stretches, before it breaks. We show that in the limit where a large enough number of transient configurations are included, the kinetics model reproduces the molecular response expected from the dynamical picture in a classical, one-trajectory sense. (C) 2002 Elsevier Science B.V. All rights reserved.

General information
State: Published
Organisations: California Institute of Technology
Contributors: Møller, K. B., Zewail, A. H.
Pages: 281-288
Publication date: 2002
Peer-reviewed: Yes

Publication information
Journal: Chemical Physics Letters
Volume: 351
Issue number: 3-4
ISSN (Print): 0009-2614
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.64 SJR 0.656 SNIP 0.61
Web of Science (2017): Impact factor 1.686
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.71 SJR 0.718 SNIP 0.689
Web of Science (2016): Impact factor 1.815
BFI (2015): BFI-level 1
Quantum dynamics for dissipative systems: A hydrodynamic perspective

General information
State: Published
Organisations: Ecole Normale Superieure
Contributors: Burghardt, I., Møller, K. B.
Pages: 7409
Publication date: 2002
Peer-reviewed: Yes

Publication information
Journal: Journal of Chemical Physics
Volume: 117
Issue number: 16
ISSN (Print): 0021-9606
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 2.5 SJR 1.252 SNIP 0.926
Web of Science (2017): Impact factor 2.843
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.13 SJR 1.486 SNIP 0.964
Web of Science (2016): Impact factor 2.965
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 1.98 SJR 1.255 SNIP 0.964
Web of Science (2015): Impact factor 2.894
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.54 SJR 1.446 SNIP 1.02
Web of Science (2014): Impact factor 2.952
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.95 SJR 1.559 SNIP 1.174
Web of Science (2013): Impact factor 3.122
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.86 SJR 1.832 SNIP 1.137
Web of Science (2012): Impact factor 3.164
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.07 SJR 1.845 SNIP 1.215
Web of Science (2011): Impact factor 3.333
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.777 SNIP 1.064
Web of Science (2010): Impact factor 2.921
Web of Science (2010): Indexed yes
Femtosecond Activation of Reactions: The Concepts of Non-ergodic Behavior and Reduced-space Dynamics

General information
State: Published
Organisations: California Institute of Technology
Contributors: Møller, K. B., Zewail, A. H.
Pages: 157-188
Publication date: 2001

Host publication information
Title of host publication: Essays in Contemporary Chemistry : From Molecular Structure towards Biology
Place of publication: Zürich
Publisher: Wiley-VCH
Editors: Quinkert, G., Kisakürek, M.
Source: orbit
Source-ID: 183481
Research output: Research › Book chapter – Annual report year: 2001

On the role of coherence in the transition from kinetics to dynamics: Theory and application to femtosecond unimolecular reactions

General information
State: Published
Organisations: Department of Chemistry
Contributors: Møller, K. B., Henriksen, N. E., Zewail, A. H.
Pages: 10477-10485
Publication date: 2000
Peer-reviewed: Yes
Comment on phase-space representation of quantum state vectors

General information
State: Published
Organisations: California Institute of Technology
Contributors: Møller, K. B.
Pages: 2531-2535
Publication date: 1999
Peer-reviewed: Yes

The concept of coherent resonances in the nuclear motion of bimolecular collisions: femtosecond probing and the classical picture
In this Letter, we report studies of coherent resonances in the course of a single bimolecular collision on the femtosecond timescale. A classical picture is presented with molecular dynamics simulations. The observed persistence of coherence elucidates the origin of the very limited spreading of the wavepacket and the crucial role of selective probing of a limited range of impact parameters. The study of this three-body system (iodine and argon) at room temperature is important for the mechanism of resonances and caging with implications for the condensed phase. (C) 1999 Elsevier Science B.V. All rights reserved.

General information
State: Published
Organisations: California Institute of Technology
Contributors: Møller, K. B., Zewail, A. H.
Pages: 1-13
Publication date: 1999
Peer-reviewed: Yes

Publication information
Journal: Chemical Physics Letters
Volume: 309
Issue number: 1-2
ISSN (Print): 0009-2614
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.64 SJR 0.656 SNIP 0.61
Web of Science (2017): Impact factor 1.686
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.71 SJR 0.718 SNIP 0.689
Web of Science (2016): Impact factor 1.815
BFI (2015): BFI-level 1
Femtosecond dynamics of transition states: the classical saddle-point barrier reactions
In this Letter, we report molecular dynamics studies of the transition state (A + BC) of saddle-point barrier reactions. We compare the theoretical findings with direct experimental observation of reaction times and kinetic energy distributions for the IHgI system. The results account for the dynamics of two- and three-body recoil from the transition state to final products and elucidate the nature of concerted (symmetric) and non-concerted (asymmetric) motions of the nuclei. (C) 1998 Published by Elsevier Science B.V. All rights reserved.
Role that separatrices and stochastic webs play in quantum dynamics

General information
State: Published
Organisations: Center for Research and Advanced Studies of the National Polytechnic Institute
Contributors: Torres-Vega, G., Møller, K. B., Zuniga-Segundo, A.
Pages: 771-780
Publication date: 1998
Peer-reviewed: Yes

Publication information
Journal: Physical Review A
Volume: 57
ISSN (Print): 2469-9926
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.46 SJR 1.288 SNIP 0.886
Web of Science (2017): Impact factor 2.909
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 2.25 SJR 1.482 SNIP 0.985
Web of Science (2016): Impact factor 2.925
Applications of classical concepts in simple quantum systems

General information
State: Published
Organisations: Department of Chemistry
Contributors: Møller, K. B.
Publication date: 1997

Publication information
Original language: English
Source: orbit
Source-ID: 222459
Research output: Research - peer-review › Journal article – Annual report year: 1998

Original language: English
Source: orbit
Source-ID: 183488
Research output: Research › Ph.D. thesis – Annual report year: 1997
Intrinsic resonance representation of quantum mechanics
The choice of basis states in quantum calculations can be influenced by several requirements, and sometimes a very
natural basis suggests itself. However often one retreats to a "merely complete" basis, whose coefficients in the
eigenstates carry Little physical insight. We suggest here an optimal representation, based purely on classical mechanics.
"Hidden" constants of the motion and good actions already known to the classical mechanics are thus incorporated into
the basis, leaving the quantum effects to be isolated and included by small matrix diagonalizations. This simplifies the
hierarchical structure of couplings between "zero-order" states. We present a (non-perturbative) method to obtain such a
basis-state as solutions to a certain resonant Hamilton-Jacobi equation. (C) 1997 American Institute of Physics.

General information
State: Published
Organisations: Physical Chemistry, Department of Chemistry, Harvard University
Contributors: Carioli, M., Heller, E., Møller, K. B.
Pages: 8564-8571
Publication date: 1997
Peer-reviewed: Yes

Publication information
Journal: Journal of Chemical Physics
Volume: 106
Issue number: 20
ISSN (Print): 0021-9606
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 2.5 SJR 1.252 SNIP 0.926
Web of Science (2017): Impact factor 2.843
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.13 SJR 1.486 SNIP 0.964
Web of Science (2016): Impact factor 2.965
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 1.98 SJR 1.255 SNIP 0.964
Web of Science (2015): Impact factor 2.894
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.54 SJR 1.446 SNIP 1.02
Web of Science (2014): Impact factor 2.952
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.95 SJR 1.559 SNIP 1.174
Web of Science (2013): Impact factor 3.122
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.86 SJR 1.832 SNIP 1.137
Web of Science (2012): Impact factor 3.164
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.07 SJR 1.845 SNIP 1.215
Web of Science (2011): Impact factor 3.333
In this article we argue that the state-vector phase-space representation recently proposed by Torres-Vega and co-workers [introduced in J. Chem. Phys. 98, 3103 (1993)] coincides with the totality of coherent-state representations for the Heisenberg-Weyl group. This fact leads to ambiguities when one wants to solve the stationary Schrödinger equation in phase space and we devise two schemes for the removal of these ambiguities. The physical interpretation of the phase-space wave functions is discussed and a procedure for computing expectation values as integrals over phase space is presented. Our formal points are illustrated by two examples. (C) 1997 American Institute of Physics.

General information
State: Published
Organisations: Physical Chemistry, Department of Chemistry, Department of Chemistry, Centro de Investigación y de Estudios Avanzados del IPN

On coherent-state representations of quantum mechanics: Wave mechanics in phase space

In this article we argue that the state-vector phase-space representation recently proposed by Torres-Vega and co-workers [introduced in J. Chem. Phys. 98, 3103 (1993)] coincides with the totality of coherent-state representations for the Heisenberg-Weyl group. This fact leads to ambiguities when one wants to solve the stationary Schrödinger equation in phase space and we devise two schemes for the removal of these ambiguities. The physical interpretation of the phase-space wave functions is discussed and a procedure for computing expectation values as integrals over phase space is presented. Our formal points are illustrated by two examples. (C) 1997 American Institute of Physics.

General information
State: Published
Organisations: Physical Chemistry, Department of Chemistry, Department of Chemistry, Centro de Investigación y de Estudios Avanzados del IPN
On wave-packet dynamics in a decaying quadratic potential

We consider the time-dependent Schrödinger equation for a quadratic potential with an exponentially decaying force constant. General analytical solutions are presented and we highlight in particular, the signatures of classical mechanics in the wave packet dynamics.
Displaced squeezed number states: Position space representation, inner product, and some applications

For some applications the overall phase of a quantum state is crucial. For the so-called displaced squeezed number state (DSN), which is a generalization of the well-known squeezed coherent state, we obtain the position space representation with the correct overall phase, from the dynamics in a harmonic potential. The importance of the overall phase is demonstrated in the context of characteristic or moment generating functions. For two special cases the characteristic function is shown to be computable from the inner product of two different DSNs.

General information
State: Published
Organisations: Physical Chemistry, Department of Chemistry, Department of Chemistry
Contributors: Møller, K. B., Jørgensen, T. G., Dahl, J. P.
Pages: 5378-5385
Publication date: 1996
Wave packet dynamics and photofragmentation in time-dependent quadratic potentials

We study the dynamics of generalized harmonic oscillator states in time-dependent quadratic potentials and derive analytical expressions for the momentum space and the Wigner phase space representation of these wave packets. Using these results we consider a model for the rotational excitation of a diatomic fragment produced in the photofragmentation of a triatomic molecule and we highlight the signatures of classical mechanics in the final product distribution of this process. (C) 1996 American Institute of Physics.
Wigner method dynamics in the interaction picture
The possibility of introducing an interaction picture in the semiclassical Wigner method is investigated. This is done with an interaction Picture description of the density operator dynamics as starting point. We show that the dynamics of the density operator dynamics as starting point. We show that the dynamics of the interaction picture Wigner function is solved by running a swarm of trajectories in the classical interaction picture introduced previously in the literature. Solving the Wigner method dynamics of collision processes in the interaction picture ensures that the calculated transition probabilities are unambiguous even when the asymptotic potentials are anharmonic. An application of the interaction picture Wigner method to a Morse oscillator interacting with a laser field is presented. The calculated transition probabilities are in good agreement with results obtained by a numerical integration of the Schrodinger equation.

General information
State: Published
Organisations: Department of Chemistry, Physical and Biophysical Chemistry
Contributors: Møller, K. B., Dahl, J. P., Henriksen, N. E.
Pages: 3272-3279
Publication date: 1994
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry
Volume: 98
Issue number: 13
ISSN (Print): 0022-3654
Ratings:
Web of Science (2010): Indexed yes
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Scopus rating (1999): SJR 1.641 SNIP 2.478
Original language: English
DOIs:
10.1021/j100064a005
Source: orbit
Source-ID: 183487
Research output: Research - peer-review → Journal article – Annual report year: 1994

Projects:

Computational Spectroscopy in Natural sciences and Engineering (COSINE): CC, ADC and DFT protocols for magnetically induced CD spectroscopies and chiral spectroscopies of excited states
Fedotov, D., PhD Student, Department of Chemistry
Coriani, S., Main Supervisor, Department of Chemistry
Møller, K. B., Supervisor, Department of Chemistry
01/09/2018 → 31/08/2021
Project: PhD

Computational Spectroscopy in Natural sciences and Engineering (COSINE): Coupled cluster methods for linear and non-linear X-ray spectroscopies, photoionisation, photodetachment and photoelectron spectroscopy
Moitra, T., PhD Student, Department of Chemistry
Coriani, S., Main Supervisor, Department of Chemistry
Møller, K. B., Supervisor, Department of Chemistry
Marie Curie (EU-stipendium)
01/09/2018 → 31/08/2021
Award relations: Computational Spectroscopy in Natural sciences and Engineering (COSINE): Coupled cluster methods for linear X-ray spectroscopies, photoionisation, photodetachment and photoelectron spectroscopy
Project: PhD

Theoretical Inorganic Chemistry
Moltved, K. A., PhD Student, Department of Chemistry
Kepp, K. P., Main Supervisor, Department of Chemistry
Detection and control of bimolecular reactions from preformed weakly bound clusters
Voute, A. P., PhD Student, Department of Chemistry
Henriksen, N. E., Main Supervisor, Department of Chemistry
Larsen, R. W., Supervisor, Department of Chemistry
Møller, K. B., Supervisor, Department of Chemistry
Institut stipendie (DTU)
01/11/2017 → 31/10/2020
Award relations: Detection and control of bimolecular reactions from preformed weakly bound clusters
Project: PhD

Novel Response Methods for Challenging Phenomena
Lopez Vidal, M., PhD Student, Department of Chemistry
Coriani, S., Main Supervisor, Department of Chemistry
Møller, K. B., Supervisor, Department of Chemistry
Institut stipendie (DTU)
15/09/2017 → 14/09/2020
Award relations: Novel Response Methods for Challenging Phenomena
Project: PhD

Katalytisk omdannelse af biomass til flydende brændsler
Kunov-Kruse, A. J., PhD Student, Department of Chemistry
Fehrmann, R., Main Supervisor, Department of Chemistry
Riisager, A., Supervisor, Department of Chemistry
Møller, K. B., Examiner, Department of Chemistry
Beato, P., Examiner
Rogers, R. D., Examiner
DTU, Samfinansiering
01/03/2010 → 19/08/2013
Award relations: Katalytisk omdannelse af biomass til flydende brændsler
Project: PhD

Undersøgelse af interaktioner mellemlectiner og sukkerarer, vha. AFM-mikrobiologi og molekylær dynamiske stimuleringer
Nygaard, T. P., PhD Student, Department of Chemistry
Peters, G. H., Main Supervisor, Department of Chemistry
Hansen, F. Y., Supervisor, Department of Chemistry
Jensen, M. Ø., Supervisor, Department of Chemistry
Møller, K. B., Examiner, Department of Chemistry
Schiøtt, H. B., Examiner
Åqvist, J. L. G., Examiner
DTU-lønnet stipendie
01/01/2004 → 26/10/2007
Award relations: Undersøgelse af interaktioner mellemlectiner og sukkerarer, vha. AFM-mikrobiologi og molekylær dynamiske stimuleringer
Project: PhD

Semi-klassiske metoder i molekylær dynamik
Møller, K. B., PhD Student, Department of Chemistry
Dahl, J. P., Main Supervisor, Department of Chemistry
Henriksen, N. E., Supervisor, Department of Chemistry
Child, M. S., Examiner
Hansen, F. Y., Examiner, Department of Chemistry
DTU-Su Stipendium, Eksperiment
01/02/1994 → 30/04/1997
Award relations: Semi-klassiske metoder i molekylær dynamik
Project: PhD
Atomistic Mechanisms of Functional Molecules
Abedi, M., PhD Student, Department of Chemistry
Møller, K. B., Main Supervisor, Department of Chemistry
Henriksen, N. E., Supervisor, Department of Chemistry
Pápai, M. I., Supervisor, Department of Chemistry
Samfinansieret - Andet
01/02/2016 → 16/05/2019
Award relations: Atomistic Mechanisms of Functional Molecules
Project: PhD

Femtochemistry and Laser Control of Photochemical Reactions
Thomas, E. F., PhD Student, Department of Chemistry
Henriksen, N. E., Main Supervisor, Department of Chemistry
Møller, K. B., Examiner, Department of Chemistry
Brixner, T., Examiner
Madsen, L. B., Examiner
Institut stipendie (DTU)
01/09/2015 → 14/10/2018
Award relations: Femtochemistry and Laser Control of Photochemical Reactions
Project: PhD

Ultrafast molecular and X-ray science: Theory and simulations
Simmermacher, M., PhD Student, Department of Chemistry
Møller, K. B., Main Supervisor, Department of Chemistry
Henriksen, N. E., Supervisor, Department of Chemistry
Coriani, S., Examiner, Department of Chemistry
Mukamel, S., Examiner
Vendrell, O., Examiner
Mukamel, S., Examiner
Vendrell, O., Examiner
Institut stipendie (DTU)
01/04/2015 → 12/11/2018
Award relations: Ultrafast molecular and X-ray science: Theory and simulations
Project: PhD

Light-induced electronic and structural dynamics
Levi, G., PhD Student, Department of Chemistry
Møller, K. B., Main Supervisor, Department of Chemistry
Dohn, A. O., Supervisor, Department of Chemistry
Henriksen, N. E., Supervisor, Department of Chemistry
Schietz, J., Examiner, Department of Physics
Chergui, M., Examiner
Gonzalez, L., Examiner
Chergui, M., Examiner
Institut stipendie (DTU)
15/12/2014 → 22/05/2018
Award relations: Light-induced electronic and structural dynamics
Project: PhD

X-ray Tracking of Electronic and Structural Dynamics During Chemical Reactions Using Free Electron Lasers
Laursen, M., PhD Student, Department of Chemical and Biochemical Engineering
Nielsen, M. M., Main Supervisor, Department of Physics
Haldrup, K., Supervisor, Department of Physics
Møller, K. B., Supervisor, Department of Chemistry
Poulsen, H. F., Examiner, Department of Physics
Feidenhans'l, R. K., Examiner, Department of Chemistry
Milne, C. J., Examiner
Feidenhans'l, R., Examiner
Milne, C. J., Examiner
Forskningsrådsfinansiering
01/11/2014 → 15/08/2018
**Structural dynamics of water solvation, studied with theoretical approaches and ultrafast X-ray methods**

Vester, P., PhD Student, Department of Physics  
Nielsen, M. M., Main Supervisor, Department of Physics  
Haldrup, K., Supervisor, Department of Physics  
Møller, K. B., Supervisor, Department of Chemistry  
Andreasen, J. W., Examiner, Department of Energy Conversion and Storage  
Abela, R., Examiner  
Larsen, S., Examiner  
Larsen, S., Examiner  
Istitut stipendie (DTU)  
15/11/2014 → 11/04/2018

**Physical Properties of Complex Chemical Systems**

Christensen, S., PhD Student, Department of Chemical and Biochemical Engineering  
Abildskov, J., Main Supervisor, Department of Chemical and Biochemical Engineering  
Møller, K. B., Examiner, Department of Chemistry  
Martin, M. G., Examiner  
Schiller, M., Examiner  
1/3 DTU-stip, 2/3 FUR/andet  
01/08/2004 → 29/08/2008

**Simulations of Transient Dynamics**

Dohn, A. O., PhD Student, Department of Chemistry  
Møller, K. B., Main Supervisor, Department of Chemistry  
Henriksen, N. E., Supervisor, Department of Chemistry  
Acevedo, O. L. L., Examiner  
Jensen, J. H., Examiner  
Jensen, J. H., Examiner  
1/3 FUU, 1/3 inst 1/3 Andet  
01/08/2011 → 17/12/2014

**Molekyldynamiske simuleringer af Lipidmembraners Vekselvirkning med Membranaktive Enzymer**

Sonne, J., PhD Student, Department of Chemistry  
Peters, G. H., Main Supervisor, Department of Chemistry  
Hansen, F. Y., Supervisor, Department of Chemistry  
Jensen, M. Ø., Supervisor, Department of Chemistry  
Møller, K. B., Examiner, Department of Chemistry  
Ipsen, J. H., Examiner, Department of Chemistry  
Marrink, S. J., Examiner  
DTU-lønnnet stipendie  
01/04/2003 → 28/08/2006

**Conical Intersections and Excited State Dynamics**

Kuhlman, T. S., PhD Student, Department of Chemistry  
Møller, K. B., Main Supervisor, Department of Chemistry  
Selling, T. I., Supervisor, Risø National Laboratory for Sustainable Energy  
Henriksen, N. E., Examiner, Department of Chemistry  
Christiansen, O., Examiner
Weber, P. M., Examiner
Sølling, T. I., Supervisor
Institut stipendie (DTU)
01/01/2010 → 19/04/2013
Award relations: Conical Intersections and Excited State Dynamics
Project: PhD

Kemisk Dynamik: Observation og kontrol
Petersen, J., PhD Student, Department of Chemistry
Møller, K. B., Main Supervisor, Department of Chemistry
Henriksen, N. E., Supervisor, Department of Chemistry
Peters, G. H., Examiner, Department of Chemistry
Engel, V., Examiner
Jørgensen, S., Examiner
DTU, Samfinansiering
01/03/2009 → 30/09/2012
Award relations: Kemisk Dynamik: Observation og kontrol
Project: PhD

Theory and Modelling of Ultrfast x-ray Imaging of Dynamical Non-Equilibrium Systems
Lorenz, U., PhD Student, Department of Chemistry
Henriksen, N. E., Main Supervisor, Department of Chemistry
Møller, K. B., Supervisor, Department of Chemistry
Hansen, F. Y., Examiner, Department of Chemistry
Engel, V., Examiner
Tschentscher, T., Examiner
DTU-lønnet stipendie
01/08/2007 → 24/11/2010
Award relations: Theory and Modelling of Ultrfast x-ray Imaging of Dynamical Non-Equilibrium Systems
Project: PhD

Sustainable Chemistry for Biomass Utilization
Lupp, D., PhD Student, Department of Chemistry
Fristrup, P., Main Supervisor, Department of Chemistry
Møller, K. B., Examiner, Department of Chemistry
Jensen, J. H., Examiner
Nørby, P., Examiner, Department of Chemistry
Jensen, J. H., Examiner
Forskningsrådssfinansiering
15/02/2012 → 30/09/2015
Award relations: Sustainable Chemistry for Biomass Utilization
Project: PhD

Study of High Pressure and High Temperature Reservoir Fluids
Varzandeh, F., PhD Student, Department of Chemistry
Yan, W., Main Supervisor, Department of Chemistry
Stenby, E. H., Supervisor, Department of Chemistry
Møller, K. B., Examiner, Department of Chemistry
Lindeloff, N., Examiner, Department of Chemical and Biochemical Engineering
Montel, F., Examiner
Eksternt finansieret virksomhed
15/12/2013 → 25/08/2017
Award relations: Study of High Pressure and High Temperature Reservoir Fluids
Project: PhD

Molecular reaction dynamics
At the fundamental level the course of chemical reactions is determined by the time-dependent Schrödinger equation. Current projects include: 1) Wave packet dynamics of nuclear motion. 2) Non-adiabatic dynamics in molecules. 3) Reaction dynamics - simple models of laser-induced dissociation dynamics. 4) Femtosecond chemistry, real-time detection of chemical reactions.
Henriksen, N. E., Project Manager, Department of Chemistry
Møller, K. B., Project Participant, Department of Chemistry
Molekylær Dynamik og Kemisk Kinetik
Ved hjælp af ultrakorte laserpulse er det i dag mulig at følge og eventuelt kontrollere det tidslige forløb af kemiske omdannelser. Formålet med dette projekt er at bygge bro mellem disciplinerne molekylær dynamik og kemisk kinetik med henblik på at udvikle et teoretisk begrebsapparat og beregningsmetoder, der kan assistere i fortolkningen af eksperimentelle observationer og i designet af nye eksperimenter.
Møller, K. B., Project Manager, Department of Chemistry
Forskningsrådene - STVF: DKK1,617,919.00
01/06/2002 → 31/05/2005
Award relations: Molekylær Dynamik og Kemisk Kinetik
Project: Research

Molecular Reaction Dynamics
Møller, K. B., Project Manager, Department of Chemistry
Forsk. Private danske - Fonde: DKK981,823.00
01/06/2005 → 31/05/2007
Award relations: Molecular Reaction Dynamics
Project: Research

Laser control of chemical reactions
The course of chemical reactions is determined by the time-dependent Schrodinger equation. The outcome of reactions can be changed by applying external fields such that the formation of unwanted products can be avoided or minimized. Current projects include: 1) Laser control of bond-selective fragmentation 2) Laser control of electronic motion
Henriksen, N. E., Project Manager, Department of Chemistry
Møller, K. B., Project Participant, Department of Chemistry
Ukendt: DKK500,000.00
01/01/1996 → …
Award relations: Laser control of chemical reactions
Project: Research

Phase Space Formulation of Quantum Mechanics
Quantum-mechanical descriptions that operate in phase space have proved very useful, both for the description of particle motion and for the description of the quantized electromagnetic field. The project includes: 1. Foundation of phase-space representations; 2. Group-theoretical aspects; 3. The dual nature of phase-space representations; 4. Wavefunctions in phase space; 5. Dynamical equations for phase-space distributions; 6. Analytical and numerical generation of phase-space distributions for oscillators, atoms and molecules; 7. Applications in molecular dynamics; 8. Applications in spectroscopy; 9. Coherent and squeezed states of the electromagnetic field. The project is partly financed by a grant from The Danish Natural Sciences Research Council (SNF).
Dahl, J. P., Project Manager, Department of Chemistry
Henriksen, N. E., Project Participant, Department of Chemistry
Møller, K. B., Project Participant, Department of Chemistry
01/01/1990 → …
Project: Research

Activities:

Photoactive transition-metal complexes: solvent and solvent-mediated dynamics
Period: 25 Jan 2019
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Degree of recognition: Local

Related event
Company seminar at Synopsys Denmark
25/01/2019 → 25/01/2019
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Ultrafast dynamics: Computer simulations and spectroscopic signatures
Period: 22 Nov 2018 → 23 Nov 2018
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Degree of recognition: International

Related event
Modern Aspects of Computational Spectroscopy
22/11/2018 → 23/11/2018
Pisa, Italy
Activity: Talks and presentations › Conference presentations

Ultrafast dynamics in photo-excited transition-metal complexes
Period: 9 Nov 2018
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Degree of recognition: National

Related event
Department of Chemistry Seminar
09/11/2018 → 09/11/2018
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Filming of bond formation and accompanying dynamics in the surroundings
Period: 23 Sep 2018 → 26 Sep 2018
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Degree of recognition: International

Related event
Intra- and inter-molecular (atomic) interactions (a MOLIM Working Group 1 meeting)
23/09/2018 → 26/09/2018
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Ultrafast photodynamics of bimetallic complexes in solution
Period: 3 Sep 2018 → 7 Sep 2018
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Degree of recognition: International

Related event
10th International Meeting on Photodynamics and Related Aspects
03/09/2018 → 07/09/2018
Cartagena, Colombia
Activity: Talks and presentations › Conference presentations

13th Nordic Femtochemistry Conference
Period: 16 Aug 2018 → 17 Aug 2018
Klaus Braagaard Møller (Organizer)
Department of Chemistry
Degree of recognition: International

Related event

13th Nordic Femtochemistry Conference
16/08/2018 → 17/08/2018
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference

Ultrafast dynamics in photo-excited transition-metal complexes
Period: 21 Jun 2018
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry

Description
Physical Chemistry Seminar

Related external organisation

Swiss Federal Institute of Technology Lausanne
CH-1015, Lausanne, Switzerland
Activity: Talks and presentations › Conference presentations

3rd MOLIM General Meeting
Period: 19 Apr 2018 → 21 Apr 2018
Klaus Braagaard Møller (Participant)
Department of Chemistry
Degree of recognition: International

Related event

3rd MOLIM General Meeting
19/04/2018 → 21/04/2018
Budapest, Hungary
Activity: Attending an event › Participating in or organising a conference

Ultrafast electronic and nuclear dynamics in photo-excited transition-metal complexes
Period: 18 Apr 2017 → 21 Apr 2017
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry

Description
CMST COST Action CM1405
Degree of recognition: International

Related event

International Workshop on Molecular Quantum Dynamics and Kinetics
18/04/2017 → 21/04/2017
Zürich, Switzerland
Activity: Talks and presentations › Conference presentations

Molecules in motion observed with X-rays
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
**Description**  
CMST COST Action CM1405

**Related event**

**2nd MOLIM General Meeting**  
10/10/2016 → 12/10/2016  
Dubrovnik, Croatia  
Activity: Talks and presentations › Conference presentations

**How to convert light to chemical energy – the initial steps**  
Period: 10 Dec 2015  
Klaus Braagaard Møller (Invited speaker)

Department of Chemistry

**Related event**

**Physical Chemistry Seminar**  
10/12/2015 → 10/12/2015  
Copenhagen, Denmark  
Activity: Talks and presentations › Conference presentations

**MOLIM General Meeting**  
Klaus Braagaard Møller (Invited speaker)

Department of Chemistry

**Description**  
Ultrafast molecular motion: experiment and simulation

CMST COST Action CM1405

**Related event**

**1st MOLIM General Meeting**  
26/08/2015 → 29/08/2015  
Paris, France  
Activity: Talks and presentations › Conference presentations

**12th International Femtochemistry Conference**  
Period: 13 Jul 2015 → 17 Jul 2015  
Klaus Braagaard Møller (Participant)

Department of Chemistry

**Description**  
Poster: Direct Dynamics Simulations of Metal Complexes in Solution for Interpretation of XFEL Results

**Related event**

**12th International Femtochemistry Conference**  
13/07/2015 → 17/07/2015  
Hamburg, Germany  
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**XFEL Symposium**  
Klaus Braagaard Møller (Invited speaker)

Department of Chemistry

**Description**
Dynamics of chemical bond formation – on the computer

Related event

XFEL Symposium
25/08/2014 → 27/08/2014
Sørup, Denmark
Activity: Talks and presentations › Conference presentations

Molecules in Motion
Period: 10 Jun 2014 → 12 Jun 2014
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry

Description
Ultrafast molecular motion: theory and experiment

Related event

Molecules in Motion
10/06/2014 → 12/06/2014
Dragør, Denmark
Activity: Talks and presentations › Conference presentations

Quantum and classical complexity
Period: 5 May 2014 → 7 May 2014
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry

Description
Chemical dynamics in complex systems.

Related event

Quantum and classical complexity: From atoms to biosystems
05/05/2014 → 07/05/2014
Bad Homburg, Germany
Activity: Talks and presentations › Conference presentations

The Copenhagen Conference on Femtochemistry
Period: 7 Jul 2013 → 12 Jul 2013
Klaus Braagaard Møller (Organizer)
Department of Chemistry
Physical and Biophysical Chemistry

Related event

The Copenhagen Conference on Femtochemistry
07/07/2013 → 12/07/2013
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising a conference

Chemical Dynamics and Spectroscopy
Period: 8 Apr 2013 → 12 Apr 2013
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Physical and Biophysical Chemistry
Related event

**Rome School on Open Systems and the Quantum-Classical Boundary**

08/04/2013 → 12/04/2013
Rome, Italy
Activity: Talks and presentations › Conference presentations

**Femtochemistry: theory and simulation**

Period: 27 May 2011
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Physical and Biophysical Chemistry

Description
Quantum Dynamics Seminar, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Related external organisation

**Unknown external organisation**
Activity: Talks and presentations › Conference presentations

**Theory and Simulation of Time-resolved X-ray Diffraction**

Period: 25 Feb 2010 → 28 Feb 2010
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Physical and Biophysical Chemistry

Related event

**Banff Meeting on Structural Dynamics**

25/02/2010 → 28/02/2010
Banff, Alberta, Canada
Activity: Talks and presentations › Conference presentations

**Theory and application of time-resolved x-ray diffraction**

Period: 2 Jun 2009 → 3 Jun 2009
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Physical and Biophysical Chemistry

Related event

**39th Danish Crystallographer Meeting**

02/06/2009 → 03/06/2009
Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

**8th Nordic Femtochemistry Meeting**

Klaus Braagaard Møller (Organizer)
Department of Chemistry
Physical and Biophysical Chemistry

Related event

**8th Nordic Femtochemistry Meeting**

02/10/2008 → 04/10/2008
Knebel, Denmark
Activity: Attending an event › Participating in or organising a conference

Chemical dynamics: Theory and simulation
Period: 2006
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Physical and Biophysical Chemistry

Related event
KAIST Lecture Series
01/01/2006 → …
Korea Advanced Institute of Science and Technology, Denmark
Activity: Talks and presentations › Conference presentations

Dissipative dynamics: Hydrodynamic and mixed representations
Period: 2006
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Physical and Biophysical Chemistry

Related event
Workshop on Dynamics of Open Quantum Systems
Bangor, Denmark
Activity: Talks and presentations › Conference presentations

Femtochemistry: Theory and simulation
Period: 2006
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Physical and Biophysical Chemistry

Related event
AMO Physics Seminar
01/01/2006 → …
University of Aarhus, Denmark
Activity: Talks and presentations › Conference presentations

Dynamics of coupled Bohmian and phase-space variables
Period: 2005
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Physical and Biophysical Chemistry

Related event
Workshop on Quantum Dynamics of Complex Molecular Systems
18/05/2005 → 20/05/2005
Paris, France
Activity: Talks and presentations › Conference presentations
Quantum hydrodynamic moment expansions: A bridge between phase space distributions and Bohmian mechanics
Period: 2004
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Physical and Biophysical Chemistry

Related event
Quantum Molecular Dynamics for Condensed Phase Applications : CECAM Workshop
16/09/2004 → 18/09/2004
Lyon, France
Activity: Talks and presentations › Conference presentations

Ultrafast IR spectroscopy of water: A theoretical study
Period: 2003
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Physical and Biophysical Chemistry

Related event
Kemisk Forenings Årsmøde
12/06/2003 → …
Odense, Denmark
Activity: Talks and presentations › Conference presentations

Trajectories in phase space: Hydrodynamics vs. Liouville space
Period: 2002
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Physical and Biophysical Chemistry

Related event
Currents, Trajectories and Applications in Quantum Dynamics: CECAM Workshop
01/01/2002 → …
Denmark
Activity: Talks and presentations › Conference presentations

Prizes:
Teacher of the Year
Klaus Braagaard Møller (Recipient)
Department of Chemistry

Details
Awarded date: 25 Apr 2008
Degree of recognition: Local
Prize: Prizes, scholarships, distinctions