Report on Workshop Symposium for Theoretical Chemistry – Large, Non-biological Systems

University of Saarland, Saarbrücken, Germany

September 16th – 20th 2007

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Organized by Michael Springborg (University of Saarland)

Web page: http://www.stc2007.uni-saarland.de

Symposium for Theoretical Chemistry – Large, Non-biological Systems

Report

The symposium for theoretical chemistry took place in Saarbrücken September 16th – 20th 2007 on the campus of the University of Saarland, Germany. It was organized by Michael Springborg (Saarbrücken) and his team (Michael Bauer, Anton Bayer, Yi Dong, Valeri Grigoryan, Hanno Kamp, Elisaveta Kasabova, Marco Schüle, Violina Tevekeliyska, Habib Ur Rehman, and Ingelore Weidenfeld). Enormous support with the organization was provided by Uta Merkle and her team at the *Kontaktstelle für Wissens- und Technologietransfer* (KWT) at the University of Saarland. The informal opening of the conference took place at a reception Sunday evening in the townhall of the town of Saarbrücken. In the official opening, Monday September 17th, it was emphasized that the symposium had become internationally recognized, whereas the first such symposia were essentially limited to the German-speaking countries. With the main topic of the symposium, large, non-biological systems, it was possible to bridge a gap between physics and chemistry, although also contributions to smaller and/or biological systems were presented. During the following 3 1/2 days 12 invited and 24 contributed talks as well as almost 170 posters were presented. The conference was organized as a low-cost conference and it was encouraging to see that many young scientists considered that a possibility to attend and also present their work. The first session was devoted to molecular-dynamics simulations. Dominik Marx (Bochum, Germany) reported about the latest developments in ab initio, molecular dynamics simulations, including presenting an approach for studying antiferromagnetic coupled spin systems. In the next two talks, Daniel Sebastiani (Mainz, Germany) reported about the calculation of momentum densities of protons and Petr Slavíček (Prague, Czech Republic) told about his studies on photochemical reactions of molecules and clusters.

The second session was opened by a talk by Richard Martin (Los Alamos, USA) who told about oxides of f electron elements. Theoretical studies of those systems are non-trivial due to strong correlation effects combined with relativistic effects. Also the presentation of Hélène Bolvin (Strasbourg, France) was devoted to heavy elements. She described an approach for calculating g matrix elements and applied it on various actinide compounds. In his talk, Anatoly Titov (St. Petersburg, Russia) discussed relations between the properties of heavy-atom molecules as calculated with 'normal' electronic-structure methods and those predicted by more fundamental approaches based on the standard model.

In his talk, John Perdew (New Orleans, USA) gave a clear overview of the 'Jacob's ladder' of density functionals, with increasingly advanced functionals on the higher rungs. LDA and GGA functionals form the first two rungs, and together with the meta-GGA functionals of the third rung they are all completely non-empirical constructions. The latest developments, the hyper-GGA functionals on the fourth rung, on the other hand, are based on an orbital-formulation of exchange energy, whereby a cancellation of errors between exchange and correlation functionals is lost and, simultaneously, one has to introduce empirical parameters. That he used 'old-fashioned' viewgraphs that even were modified 'on the fly' added to the interest that his talk arouse. In two further talks, by Kartick Gupta (University of Burdwan, India) and Laszlo von Szentpaly (Stuttgart, Germany), methods for using descriptors to study chemical acitivities of individual molecules were discussed.

Poul Jørgensen (Århus, Denmark) and Christian Ochsenfeld (Tübingen, Germany) presented methods that allowed for efficient theoretical treatments of very large systems. With these methods also larger fragments of a DNA molecule could be treated (with more than 1000 atoms and 10000 basis functions). Subsequently, Andreas Köhn (Mainz, Germany) discussed the transfer of excitation energies between donor and acceptor molecules. Andreas Köhn presented an accurate approach for the theoretical study of these processes.

In the last talk on the first day of the symposium, Benoît Champagne (Namur, Belgium) presented methods and results for the calculation of structural, mechanical, electronic, and optical properties of regular polymers. He showed that an approach based on periodicity is much more efficient than one based on finite systems of increasing size.

Monday evening was devoted to the first poster session. During some three hours halfpart of the posters was presented and intensively discussed. To the pleasure of the organizers, the larger part of the attendees stayed at the symposium also during the evening.

Tuesday morning was reserved for the presentation of the Hellmann award winner, Andreas Dreuw (Frankfurt/Main, Germany). After having received his award, he presented his work on photoinduced electron transfer in biochemical systems. Subsequently, Serguei Fomine (Mexico City, Mexico) presented theoretical predictions for the properties of tubular systems of oligothiophenes. In her talk, Alisa Krishtal (Antwerp, Belgium) analysed in detail methanol clusters with the ultimate purpose of understanding how the macroscopic properties of a solvent (i.e., methanol) depend on the microscopic properties of the solvent molecules.

Benedetta Mennucci (Pisa, Italy) discussed the most recent extensions of the polarizable continuum method for the study of molecules in solution. Within one extension, also excited states can be treated. She pointed out the srengths and limitations of the different methods for treating solvated molecules. Jan-Ole Joswig (Dresden, Germany) used a parameterized density-functional method in studying proton transport in polyphosphonic acids that are considered interesting materials for fuel cells. Dipole switching processes in large molecules was the topic of the presentation of Tillmann Klamroth (Potsdam, Germany).

Catalytic properties of surfaces of oxides were discussed by Joachim Sauer (Berlin, Germany). He demonstrated how a close collaboration with experimentalists can be very useful in obtaining a detailed understanding of the materials properties. Dynamical properties were studied by Judith Voll (Munich, Germany), who considered laser induced dynamics of β-carotene using a simplified model. Ozlem Ozcan (Düsseldorf, Germany) presented his results of Monte Carlo – density-functional studies of the adsorption of organosilanes on a ZnO surface.

Arne Lüchow (Aachen, Germany) discussed advantages (accuracy) and disadvantages (limited size of the treatable systems) of quantum Monte Carlo simulations and gave also examples of his most recent applications of this approach. Chemical reactions was the topic of the presentation of Vincent Tognetti (Paris, France) who studied a catalytic process of ethylene dimerization. Philipp Scherer (Munich, Germany) exploited in detail a simple model system for the study of electron transfer processes in large biological systems.

Before the second poster session, Frank-Dieter Kuchta of the German Research Council (DFG) gave a very useful overview of the activities of DFG and of the different programs of this funding agency. After the dinner, the second halfpart of the posters was presented, and, as at the first poster session, this poster session was very well attended.

In the first talk on Wednesday morning, Karlheinz Schwarz (Vienna, Austria) presented the latest developments of the WIEN2k computer programs for the study of crystalline materials. This included also recent applications, where, e.g., the LDA+U approach was used to get a proper description of the materials. By combining information from more different types of experiment, the value of the parameter U could be settled quite accurately. In another application, he showed that also surfaces can be studied. This included an impressive example of a borazine nanomesh on the Rh(111) surface whose structure was accurately determined. A perfect agreement with experimental observables was obtained, although the interpretation differed. This system contained about 1100 atoms per unit cell.

David Benoit (Ulm, Germany) presented a new method for the calculation of vibrational properties of large systems. Since these properties are important for the characterization of the systems, such theoretical developments are very useful in providing links between theory and experiment. Liviu Hozoi gave results for the study of extended systems were correlation effects were added with the so called local methods to a Hartree-Fock based calculation.

The second morning session on Wednesday was devoted to larger, but finite systems. First, David Wales (Cambridge, UK) discussed ways of describing and determining the ‘energy landscapes’ of such systems, i.e., the total-energy hypersurfaces. The so called disconnectivity graphs provide a useful two-dimensional presentation of the hypersurfaces that also allow for analysing how easily a local or global total-energy minimum can be reached. Subsequently, Konstantin Neyman (Barcelona, Spain) and Christoph Scheurer (Munich, Germany) discussed the properties of different specific nanoparticles.

Wednesday afternoon was devoted to an excursion were a couple of interesting places in Saarland were visited. These were the Saar Loop where the river Saar makes a spectacular 180° turn as well as the iron work in Völkingen that is a Unesco World Cultural Heritage. The day closed with a conference dinner at the university.

The last day of the symposium, Thursday, started with a presentation by Martin Kaupp (Würzbung, Germany) who shared his time between two topics, the theoretical determination of NMR parameters and the development of new hybrid density functionals where the hybrid parameter was allowed to be position dependent. In his talk, Dominik Kröner (Potsdam, Germany) presented a theoretical study of the laser control of the switching of a chiral molecule. Due to the complexity of the problem at hand, the calculations were based on a simplified model. Subsequently, Wolfgang Eisfeld (Bielefeld, Germany) discussed the results of extensive calculations on a small molecule, NO_3, where also all vibrational degrees of freedom were included in the dynamical simulations.

The last session of the symposium was devoted to crystalline compounds. Hermann Stoll (Stuttgart, Germany) discussed his approach for splitting correlation into a long- and a short-ranged part that can be treated separately. The short-ranged parts are treated with density functional methods, and the long-ranged parts with wavefunction based methods. Ultimately, this leads to a highly accurate method. Beate Paulus (Dresden, Germany) applied the method of local increments for the inclusion of correlation effects to study the adsorption of CO on a ceria surface. Finally, Ulrich Wedig (Stuttgart, Germany) demonstrated that even some crystal structures of some elements (Zn and Cd) are not well understood.

In total the conference demonstrated that the field of computational materials science / chemistry / physics is very active and that methodological developments have made it possible to apply computational approaches to the study of systems and situations that accurately match those found in experiment, and not only idealized model system. Thereby, such calculations have become truely predictive. Although also the development in computer technology has been of paramount importance, the most significant improvements have been obtained through improved computational and theoretical methods.

The developments that have made it possible to use computational approaches predictively include the treatment of dynamical properties of larger systems, methods for studying systems in realistic atmospheres and solutions, the study of chemical reactions in gas phase and on catalytic surfaces, and the possibility of studying structural and electronic properties of large, but finite, nanosystems. But also the development of highly accurate density functionals in density-functional theory and of alternative methods for studying certain systems at a more accurate level remains being very important for assuring that results obtained with theoretical methods become increasingly accurate and reliable.

The systems that were presented during the symposium represented an impressive range from crystalline or biological systems with more than 1000 atoms being treated explicitly, to the study of dynamical properties in materials of relevance for the development of fuel cells. The calculation of all kinds of response functions provided a close link to experimental studies.

Finally, further information on the symposium, including pictures taking during the 3 1/2 days, can be found on the homepage of the symposium, http://www.stc2007.uni-saarland.de, at least until the end of the year 2007.

Saarbrücken, October 2007, Michael Springborg

Programme

Sunday, September 16th

Reception

17.00 – 20.00	Registration in the Town Hall of the Town of Saarbrücken
18.00 – 20.00	Reception in the Town Hall of the Town of Saarbrücken

Monday, September 17th

From 07.45	Registration in front of the lecture hall

Session 1

Chair:	*Gernot Frenking (Marburg, Germany)*
08.30 – 08.35	Michael Springborg (Saarbrücken, Germany): *Opening*
08.35 – 09.20	I1: Dominik Marx (Bochum, Germany): *Recent trends in ab initio simulation*
09.20 – 09.40	C1: Daniel Sebastiani (Mainz, Germany): *Proton momentum-space densities from first-principles path-integral molecular dynamics simulations*
09.40 – 10.00	C2: Petr Slavíček (Prague, Czech Republic): *Photochemical reactions studied by ab initio quantum molecular dynamics: from molecules to clusters*
10.00 – 10.30	Break

Session 2

Chair:	*Christoph van Wüllen (Berlin, Germany)*
10.30 – 11.15	I2: Richard L. Martin (Los Alamos, USA): *The localization / delocalization dilemma in the electronic structure of f-element oxides*
11.15 – 11.35	C3: Anatoly Titov (St. Petersburg, Russia): *Combined ab initio methods and accurate study of heavy-atom molecules to search for new physics beyond the standard model*
11.35 – 11.55	C4: Hélène Bolvin (Strasbourg, France): *Calculation of electronic g-matrices of actinide compounds*
11.55 – 13.30	Lunch break

Session 3

Chair: *W. H. Eugen Schwarz (Siegen, Germany)*

13.30 – 14.15 I3: John P. Perdew (New Orleans, USA): *Hyper-generalized gradient approximation for the exchange-correlation energy of density functional theory*

14.15 – 14.35 C5: Kartick Gupta (Bishnupur, India): *A DFT study of acidity of ortho- and para-substituted aromatic acids using molecular descriptors*

14.35 – 14.55 C6: Laszlo von Szentpaly (Stuttgart, Germany): *Critique and correction of conceptal DFT*

14.55 – 15.30 Break

Session 4

Chair: *Christel Marian (Düsseldorf, Germany)*

15.30 – 16.15 I4: Poul Jørgensen (Århus, Denmark): *A ground-state directed optimization scheme for the Kohn-Sham energy*

16.15 – 16.35 C7: Christian Ochsenfeld (Tübingen, Germany): *A linear-scaling AO-based MP2 method for large molecules by rigorous integral estimates*

16.35 – 16.55 C8: Andreas Köhn (Mainz, Germany): *Excitation energy transfer rates from correlated transition densities*

16.55 – 17.45 Break

Session 5

Chair: *Thomas Heine (Dresden, Germany)*

17.45 – 18.30 I5: Benoît Champagne (Namur, Belgium): *Ab initio polymer quantum theory: structural and vibrational properties*

18.30 – 19.30 Dinner

Poster Session 1

19.30 – 22.00 Posters with odd numbers. (Including free beverages)

Tuesday, September 18th

From 08.35	Registration in front of the lecture hall

Session 6

Chair:	*Wolfgang Domcke (Munich, Germany)*
08.35 – 09.20	Presentation of the Hellmann Prize winner
09.20 – 09.40	C9: Serguei Fomine (Mexico City, Mexico): *Tubular aggregates of cyclic oligothiophenes. A theoretical study*
09.40 – 10.00	C10: Alisa Krishtal (Antwerp, Belgium): *The effect of structural parameters on the polarizabilities of methanol clusters: a Hirshfeld study*
10.00 – 10.30	Break

Session 7

Chair:	*Gotthard Seifert (Dresden, Germany)*
10.30 – 11.15	I6: Benedetta Mennucci (Pisa, Italy): *Structure and properties of molecular solutes in electronic excited states: a quantum mechanical Polaizable Continuum Model*
11.15 – 11.35	C11: Jan-Ole Joswig (Dresden, Germany): *Proton transport in liquid phosphonic acid and polyphosphonic acid based polymers studied with molecular-dynamics simulations*
11.35 – 11.55	C12: Tillmann Klamroth (Potsdam, Germany): *Explicitly time-dependent configuration interaction simulations: dipole switching in large molecules*
11.55 – 13.30	Lunch break

Session 8

Chair:	*Georg Jansen (Essen, Germany)*
13.30 – 14.15	I7: Joachim Sauer (Berlin, Germany): *Structure and reactivity of oxide catalysts*
14.15 – 14.35	C13: Judith Voll (Munich, Germany): *Laser induced femtosecond dynamics in the excited states of beta-carotene*
14.35 – 14.55	C14: Ozlem Ozcan (Düsseldorf, Germany): *A Monte Carlo – DFT study: adsorption of organosilanes on polar ZnO(0001) surfaces*
14.55 – 15.30	Break

Session 9

Chair:	*Dirk Andrae (Bielefeld, Germany)*
15.30 – 16.15	I8: Arne Lüchow (Aachen, Germany): *Electron structure quantum Monte Carlo:recent developments and applications*
16.15 – 16.35	C15: Vincent Tognetti (Paris, France): *DFT study of ethylene dimerization by mixed bidentate P–N nickel complexes*
16.35 – 16.55	C16: Philipp Scherer (Munich, Germany): *Nonadiabatic coupling mechanism for ultrafast electron transfer in the reaction center of bacterial photosynthesis*
16.55 – 17.30	Break

Session X

Chair:	*Wolfgang Domcke (Munich, Germany)*
17.30 – 18.00	X: Frank-Dieter Kuchta (DFG, Germany): *Die Deutsche Forschungsgemeinschaft informiert!*
18.00 – 18.30	Mitgliederversammlung AGTC
18.30 – 19.30	Dinner

Poster Session 2

19.30 – 22.00	Posters with even numbers. (Including free beverages)

Wednesday, September 19th

From 08.35	Registration in front of the lecture hall

Session 10

Chair:	*Daniel Sebastiani (Mainz, Germany)*
08.35 – 09.20	I9: Karlheinz Schwarz (Vienna, Austria): *DFT calculations of crystals and surfaces with WIEN2k*
09.20 – 09.40	C17: David Benoit (Ulm, Germany): *Accurate computation of vibrational spectra for extended systems*
09.40 – 10.00	C18: Liviu Hozoi (Dresden, Germany): *Correlated bands in oxides with wave-function based methods*
10.00 – 10.30	Break

Session 11

Chair:	*Beate Paulus (Dresden, Germany)*
10.30 – 11.15	I10: David Wales (Cambridge, UK): *Energy landscapes: from clusters to biomolecules*
11.15 – 11.35	C19: Konstantin Neyman (Barcelona, Spain): *Nanosized metal and oxide particles as realistic models of catalytic materials*
11.35 – 11.55	C20: Christoph Scheurer (Munich, Germany): *Simulation of photoluminescence spectra of neutral and charged exciton states in self-assembled semiconductor quantum dot molecules*
12.00 – 19.30	Excursion
19.30 – ?	Conference Dinner

Thursday, September 20th

From 08.35 Registration in front of the lecture hall

Session 12

Chair: *Frank Neese (Bonn, Germany)*

08.35 – 09.20 I11: Martin Kaupp (Würzburg, Germany): *Magnetic properties and local hybrid functionals*

09.20 – 09.40 C21: Dominik Kröner (Potsdam, Germany): *Laser-controlled chiral molecular switch: Quantum simulations for the stereoselective transformation between achiral and chiral atropisomers*

09.40 – 10.00 C22: Wolfgang Eisfeld (Bielefeld, Germany): *Taming of a beast: Multimode nonadiabatic excited state dynamics in* NO_3

10.00 – 10.30 Break

Session 13

Chair: *Michael Bühl (Mühlheim, Germany)*

10.30 – 11.15 I12: Hermann Stoll (Stuttgart, Germany): *Long-range correlation and local increments*

11.15 – 11.35 C23: Beate Paulus (Dresden, Germany): *Adsorption energy calculations with the method of increments: application to the adsorption of CO on the* CeO_2*(110) surface*

11.35 – 11.55 C24: Ulrich Wedig (Stuttgart, Germany): *Bonding properties in elemental Zn and Cd*

Closing

Chair: *Michael Springborg (Saarbrücken, Germany)*

11.55 – 12.15 Anne-Marie Kelterer (Graz, Austria): Presentation of the 44th Symposium for Theoretical Chemistry, 2008

Poster Prize Board: Presentation of the winners of the poster prizes

Closing

Lunch

Departure

Abstracts of invited lectures

Recent Trends in Ab Initio Simulation

Dominik Marx[1]

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Ab initio simulation is a general class of approaches to computer simulation where the electronic structure problem is solved concurrent to the simulation. This can be achieved in molecular dynamics or Monte Carlo sampling frameworks, Car-Parrinello propagation in conjunction with density functional theory being a very efficient algorithm to do so which gives direct access to dynamical information of condensed phase systems.

This lecture will review recent developments in the field of ab initio simulation such as approximate quantum dynamics for computing the time evolution of anharmonic many-body systems and multideterminant propagation schemes for treating antiferromagnetically coupled spin systems. The former can be exploited to assess quantum effects on infrared spectra, whereas the latter allows one to address issues in molecular magnetodynamics. In addition, some representative applications will be discussed.

General References to ab initio simulation:

[1] J. Grotendorst, S. Blügel, and D. Marx (Editors), Computational Nanoscience: Do It Yourself! (NIC Jülich, 2006); see *www.theochem.rub.de/go/cprev.html*

[2] J. Grotendorst, D. Marx, and A. Muramatsu (Editors), Quantum Simulations of Complex Many-Body Systems: From Theory to Algorithms (NIC Jülich, 2002); see *www.theochem.rub.de/go/cprev.html*

The localization/delocalization dilemma in the electronic structure of f-element oxides

R.L. Martin[1]

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The electronic structure of many of the oxides containing f-elements has long been a challenge for theory. For example, the traditional workhorses of density functional theory, the local density approximation (LDA) and the generalized gradient approximations (GGA), predict many of these systems to be metallic, when in fact they are insulators with band gaps of several eV. These problems reflect the localization/delocalization dilemma faced in systems with weak overlap and seem to be largely overcome by the new generation of *hybrid* density functionals developed for molecular studies. Only recently has it been possible to apply these functionals to solids, but in the cases studied thus far we find a distinct improvement. The hybrid functionals predict the correct insulating ground state, band gap, lattice constant and magnetic behavior at 0K, where known. I will review the origin of the problem, how hybrid functionals differ from traditional ones, and recent applications to CeO_2 and Ce_2O_3, UO_2, and PuO_2, Pu_2O_3 and $PuO_{2.25}$.

Hyper-Generalized Gradient Approximation for the Exchange-Correlation Energy of Density Functional Theory

John P. Perdew,[1] Viktor N. Staroverov,[2] Jianmin Tao,[3] and Gustavo E. Scuseria[4]

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In the density functional theory of Kohn and Sham 1965 [1], the ground-state electron density and energy can be found by solving one-electron selfconsistent Schroedinger equations. In practice, the density functional for the exchange-correlation energy must be approximated. Common approximations can be arranged on the rungs of a ladder according to the ingredients used to construct the energy density. The first rung or local spin density approximation [1] uses only the local spin densities. The second rung or generalized gradient approximation (GGA) [2] uses also the gradients of the spin densities. The third rung or meta-GGA [3] uses additionally the orbital kinetic energy densities for each spin. The addition of more ingredients permits the satisfaction of more exact constraints, with greater accuracy. The first three rungs have fully nonempirical constructions [1-3]. The fourth rung or hyper-GGA uses in addition the exact exchange energy density, and is able to satisfy many more exact constraints (full exact exchange, freedom from self-interaction error, etc.). However, it loses the automatic cancellation of error between approximate exchange and approximate correlation, and so requires the use of one or more empirical parameters. We present a new hyper-GGA that satisfies essentially all the exact constraints that a hyper-GGA can, and achieves high accuracy for atomization energies of molecules and energy barriers to chemical reactions.

[1] W. Kohn and L.J. Sham, Phys. Rev. **140**, A1133 (1965).

[2] J.P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. **77**, 3865 (1996).

[3] J. Tao, J.P. Perdew, V.N. Staroverov, and G.E. Scuseria, Phys. Rev. Lett. **91**, 146401 (2003).

A Ground-State Directed Optimization Scheme for the Kohn–Sham Energy

Stinne Høst,[1] Branislav Jansík,[1] Jeppe Olsen,[1] Poul Jørgensen,[1] Simen Reine,[2] and Trygve Helgaker[2]

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Kohn–Sham density-functional calculations are used in many branches of science to obtain information about the electronic structure of molecular systems and materials. The traditional method for optimizing the Kohn–Sham energy consists of a Roothaan-Hall (RH) diagonalization of the Kohn-Sham matix to obtain a new density matrix followed by an averaging of this density matrix and the density matrices from previous iterations to obtain an improved density matrix for the next iteration. The improved density matrix is usually found using the DIIS algorithm of Pulay. The RH/DIIS method suffers from fundamental problems that may lead to divergence or, even worse, convergence to an energy saddle point rather than to the ground-state minimum. This happens in particular, for the larger and more complicated electronic systems that are often studied by Kohn–Sham theory nowadays.

We here present a novel method for Kohn–Sham energy minimization that does not suffer from the flaws of the conventional approach, combining reliability and efficiency with linear complexity. In particular, the proposed method converges to a minimum, avoiding the sometimes spurious solutions of the traditional method and bypassing the need to examine the structure of the provided solution.

Ab Initio Polymer Quantum Theory: Structural and Vibrational Properties

Benoît Champagne[1]

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Crystal orbital techniques based on periodic boundary conditions are a convenient way to describe the properties of stereoregular polymers [1]. Over the last 40 years, methods and algorithms have been elaborated at different levels of approximation, encompassing the reference Hartree-Fock level, Möller-Plesset perturbation theory, and more recently coupled-cluster approaches. This talk will review basic aspects of such approaches including lattice summations and long-range interactions, integration procedures, and quasi-linear dependencies. It will then concentrate on structural, vibrational, and mechanical properties and in particular it will discuss methods to compute the forces on nuclei, the Young elastic modulus, vibrational frequencies and intensities, as well as vibrational polarizabilities.

[1] B. Champagne, in Molecular Simulation Methods for Predicting Polymer Properties, edited by V. Galiatsatos (Wiley & Sons, New York, 2005), 1-46.

Structure and properties of molecular solutes in electronic excited states: a quantum mechanical Polarizable Continuum Model

Benedetta Mennucci [1]

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The desciption of structures and properties of electronically excited states of molecular systems is a rather complex problem. In the years, the development of linear response approaches such as CIS, ZINDO and, more recently, TDDFT has contributed to make these studies possible also for realistic systems.

In parallel to this progress in the quantum mechanical description of the electronic states there has been a parallel extension of these studies to molecules embedded in different environments of various complexity, from standard solvents to interfaces between gas and solvent or between solvent and solvent, and to metal surfaces.

In this talk a review of the most recent advances in the field obtained by exploiting a polarizable continuum model [1] is presented and discussed.

[1] J. Tomasi, B. Mennucci, and R. Cammi Chem. Rev. **105**, 2999 (2005).

Structure and Reactivity of Oxide Catalysts

Joachim Sauer[1]
[1] *Institut für Chemie, Humboldt-Universität zu Berlin, Unter den Linden 6, 10099 Berlin, Germany*

The use of computational techniques based on quantum mechanics in concert with experimental techniques for understanding the structure and reactivity of complex solid catalysts is described. The discussion for metal oxide catalysts, in particular supported transition metal oxides [1,2] and zeolites [3], includes use of quantum mechanics and statistical mechanics to bridge the gap between ultra-high vacuum model systems (surface science) and catalysts under "real" conditions [4,5]; use of quantum mechanics and IR spectroscopy to analyse the differences and similarities of gas phase clusters and solid catalysts [1,6]; limits and merits of periodic models and (embedded) cluster models; the power of DFT and needs to go beyond DFT (multi-reference, dispersion); the use of hybrid techniques: QM:MM and QM:QM [3].

[1] J. Döbler, M. Pritzsche, and J. Sauer, *J. Am. Chem. Soc.*, 2005, **127**, 10861.

[2] X. Rozanska, R. Fortrie, and J. Sauer, *J. Phys. Chem. C*, 2007, **111**, 6041.

[3] C. Tuma and J. Sauer, *Phys. Chem. Chem. Phys., 2006*, **8**, 3955.

[4] J. Weissenrieder, S. Kaya, J.-L. Lu, H.-J. Gao, S. Shaikhutdinov, H.-J. Freund, M. Sierka, T. K. Todorova, and J. Sauer, *Phys. Rev. Lett., 2005*, **95**, 0761031.

[5] M. Sierka, T. K. Todorova, S. Kaya, D. Stacchiola, J. Weissenrieder, J. Lu, H. Gao, S. Shaikhutdinov, H.-J. Freund and J. Sauer, *Chem. Phys. Lett.*, 2006, **424**, 115.

[6] S. Feyel, D. Schröder, X. Rozanska, J. Sauer and H. Schwarz, *Angew. Chem., Int. Ed.*, 2006, **45**, 4677; *Angew. Chem.*, **118**, 4793-4797.

Electron structure quantum Monte Carlo: recent developments and applications

A. Lüchow,[1]
[1] *Institut für Physikalische Chemie, RWTH Aachen University, Aachen, Germany*

With Monte Carlo techniques the numerical quantum simulation of the full-dimensional Schrödinger equation is a viable and favorably scaling method that directly, without the expansion into orbitals, describes the electron correlation. Over the last few years, these quantum Monte Carlo (QMC) methods have shown to be applicable to a wide range of quantum chemical problems with high accuracy, including excited states and weak interactions. QMC can retain the inherent favorable scaling of Monte Carlo methods in these applications. Recent applications and improvements of QMC are discussed. An addition, new ways to control the fixed-node error of the diffusion quantum Monte Carlo method are presented.

Die Deutsche Forschungsgemeinschaft informiert!

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Das Ziel dieser Veranstaltung ist es, Ihnen aktuelle Informationen aus der Forschungsförderung der Deutschen Forschungsgemeinschaft zu vermitteln. Neben allgemeinen Hinweisen zu den koordinierten DFG-Programmen, insbesondere Schwerpunkten, Förderinstrumenten für Nachwuchswissenschaftler und internationale Kooperationsprojekten, stehen Themen im Mittelpunkt, die für ihr Fachgebiet, die Theoretische Chemie, von Interesse sind. Es ist zudem vorgesehen über die Antrags- und Bewilligungsentwicklung in der Einzelförderung, die Fachgutachterwahlen 2007, die Arbeit der Fachkollegien und das Begutachtungsverfahren zu berichten.

DFT calculations of crystals and surfaces with WIEN2k

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Density functional theory (DFT) made it possible to calculate the electronic structure of rather large systems. Various functionals (LDA, GGA, hybrid functionals, LDA+U) are used to provide a proper description of the electronic strucuture of different materials. The translational symmetry of a crystal allows to focus on a unit cell but surfaces can be treated as well using periodic boundary conditions and assuming a slab geometry with an atom-free region representing vacuum. Plane waves are a natural basis set for solids but they can not represent the oscillating wave functions near a nucleus. Therfore mixed basis schemes such as the linearized augmeted plane wave (LAPW) method provide a very accurate description for all elements in the periodic table. In LAPW the unit cell is partitioned into non-overlapping atomic spheres and an interstitial region, where plane waves are used. Inside each atomic sphere the plane waves are augmented by atomic-like functions with (numerically calculated) radial functions times spherical harmonics. In addition relativistic effects and the treatment of semi-core states can be included.

The WIEN2k computer package (see www.wien2k.at) is based on this method and is one of the most accurate code for solids (for a review see [1]). Presently it is used worldwide by more than 1100 groups in academia and industry. The concepts will be described and various applications will be given from minerals to magnetic materials or metal insulator transitions, or electric field gradients.

A recent application of WIEN2k is our study of a boron nitride surface layer that forms on a metal substrate [2]. When borazine is deposited on transition metal surfaces, in particular on Rh(111), an ordered structure, called nanomesh, forms that has a periodicity of about 3.2 nm. In order to simulate this surface structure a unit cell containing about 1100 atoms is used. Nowadays such calculations are feasible and the corresponding computer requirements will be sketched. This example will be used to illustrate the various possibilities of WIEN2k calculations using forces on the atoms, geometry optimizations, densities of states, workfunctions, spectra, etc.

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Energy Landscapes: from Clusters to Biomolecules

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Coarse-graining the potential energy surface into the basins of attraction of local minima, provides a computational framework for investigating structure, dynamics and thermodynamics in molecular science [1,2]. Steps between local minima form the basis for global optimisation via basin-hopping [3,4] and for calculating thermodynamic properties using the superposition approach [1,5] and basin-sampling [6]. To treat global dynamics we must include transition states of the potential energy surface, which link local minima via steepest-descent paths. We may then apply the discrete path sampling method, which provides access to rate constants for rare events [7-9]. In large systems the paths between minima with unrelated structures may involve hundreds of stationary points of the potential energy surface. New algorithms have been developed for both geometry optimisation [10] and making connections between distant local minima [11], which allow us to treat such systems. Kinetic analysis of large stationary point databases is facilitated by a new graph transformation approach [12].

Applications will be presented for a wide variety of atomic and molecular clusters, including systems bound by isotropic interatomic potentials such as the Lennard-Jones and Morse forms, clusters of dipolar spheres [13], and molecular clusters such as nanodroplets of water [14-16]. Results for folding, misfolding and aggregation of peptides and proteins illustrate how experimental time and length scales can now be addressed for such systems.

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Magnetic Properties and Local Hybrid Functionals

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Recent advances in development, validation, and application of DFT in the area of magnetic resonance parameters are reported, based on the ReSpect program system [1]. Spin-orbit effects have important consequences on NMR and EPR parameters. One example is the unusually large spin-orbit effects on Cu hyperfine couplings in blue-copper protein sites [2]. Higher-order spin-orbit effects may be included within a spin-polarized two-component framework [3]. The computation of NMR chemical shifts of paramagnetic systems has recently been extended to systems with arbitrary spin multiplicity, by incorporating the influence of zero-field splittings on the Boltzmann distribution of energy levels [4]. Shortcomings of the existing exchange-correlation functionals become particularly apparent when looking at the NMR/EPR parameters of transition metal systems. This has motivated us to develop new functionals within the "local hybrid" framework using position-dependent exact-exchange admixture [5]. The first results are very encouraging for both thermochemistry and kinetics. In addition, the first self-consistent implementation as "localized local hybrid potentials" has allowed the first calculations of NMR chemical shifts, with equally encouraging results [6].

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Long-range correlation and local increments

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DFT is nowadays the method of choice for large molecules and extended systems, but standard LDA, GGA, and meta-GGA functionals have problems for van der Waals interaction and do not allow for a systematic improvement.

Part of these weaknesses can be overcome by restricting DFT to a short-range interelectronic interaction and using wavefunction-based ab-initio methods for the complementary long-range terms. It is shown that a both accurate and efficient treatment is possible at intermediate values of the coupling constant [1,2].

Still, application to extended systems necessitates a local correlation treatment on the ab-initio side. One of the simplest devices is a many-body expansion in terms of correlation contributions from localized orbital groups. Such an incremental expansion, on top of HF calculations, has proven to yield reliable results, at moderate cost, for a variety of solids (van der Waals crystals, ionic systems, semiconductors, and even metals) [3,4]. A possible application of the incremental method within a mixed DFT / ab-initio scheme will be discussed.

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Abstracts of contributed lectures

Proton Momentum-space Densities from First-Principles Path-Integral Molecular Dynamics Simulations

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We present an approach to compute reciprocal space probability densities of light nuclei in complex condensed-phase systems, in particular the momentum density $n_{\mathrm{nuc}}(k) = |\Psi_{\mathrm{nuc}}(k)|^2$ of protons. This property reflects the quantum nature of the hydrogen wavefunction in terms of the spatial localization and delocalization. Naturally, the momentum density of a nucleus reacts to changes in its chemical environment, especially hydrogen bonding. Momentum-space densities $n_{\mathrm{nuc}}(k)$ can directly be measured via inelastic Neutron Compton Scattering techniques.

Our method is based on finite-temperature path-integral Car-Parrinello molecular dynamics simulations. In order to obtain momentum-space densities, a modified version of the path-integral technique is used, which relies on linear ("open") paths for the particles of interest. The method is benchmarked on test systems and small molecules, and further applied to describe the ferroelectric and paraelectric states in potassium dihydrogen phosphate (KDP) at different temperatures. In such systems, the momentum distributions $n_{\mathrm{nuc}}(k)$ allow for a distinction between temperature-induced hopping and quantum tunneling states of the hydrogen-bonded protons.

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Photochemical reactions studied by *ab initio* quantum molecular dynamics: From molecules to clusters

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In the *ab initio* molecular dynamics approach, the equations of motion for both electrons and nuclei are solved simultaneously as the simulation proceeds (direct dynamics). This approach represents a hopeful tool for revealing reaction mechanisms: the dynamical equations are automatically leading us to important structures without any bias or prejudice while bond breaking or bond making processes are properly described. In many important cases the nuclear equations of motion have to include quantum effects. Specifically, quantum (or at least semiclassical) dynamics has to be employed for a description of non-adiabatic processes or when tunneling of light particles is involved. This is almost always the case in photochemistry. Full Multiple Spawning (FMS) method [1] is one route for this connection between quantum molecular dynamics and electronic structure calculations. Methods eof extedning the scope of this approach beyond simple molecules will be discussed [2].

We will show how a combination of quantum chemical and ab initio quantum dynamical calculations can be used for an exploration of photochemical reactions involving non-adiabatic processes. Two molecular examples will be provided: photochemistry of glycine [3] and photochemistry of nitrophenols.

Many important photochemical processes occur in the bulk phase or on the surface of nano-sized particles. Information obtained by a study of isolated molecules can thus be of a limited relevance. Recently, we have started to study photochemistry of molecules assembled in molecular cluster in a close collaboration with an experimental group. Two examples will be shown: study of photochemistry of pyrrole molecular clusters [4] and study of hydrogen halide acidic and photochemical dissociation on the surface of water clusters [5].

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Combined *ab initio* methods and accurate study of heavy-atom molecules to search for new physics beyond the Standart model

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The search for the space (P) and time-reversal (T) parity nonconservation effects is of fundamental importance for modern theory of fundamental interactions and symmetries and immense experimental effort is invested in the search for the fingerprints of P,T-parity nonconservation effects, such as the electron electric dipole moment (*e*EDM) [1]. The tightest bound on the value of *e*EDM, d_e, was obtained in the experiment on Tl atom, which established an upper bound of $|d_e| < 1.6 \times 10^{-27} e\cdot\text{cm}$ (e is the charge of the electron). Molecular systems provide a way for much enhanced sensitivity since the effective intra-molecular electric field acting on electrons in polar molecules can be five or more orders of magnitude higher than the maximal field available in a laboratory. Such experiments were successfully performed so far only on the molecular YbF beam. Recently some new approaches were suggested, such as the search for P,T-odd effects in molecular cations PbO* [2], HI^+, HfF^+ etc. [3]. The new generation of *e*EDM experiments will have a sensitivity of $10^{-30} \div 10^{-28} e\cdot\text{cm}$. Their results are expected to dramatically influence all the popular extensions of the Standard model, in particular supersymmetry, even if bounds on the P,T-odd effects compatible with zero are obtained [1]. For preparation and interpretation of these experiments, accurate calculations of electronic densities on the heavy nuclei are required and different molecular properties should be computed.

Precise calculations of core properties in heavy-atom systems, like to hyperfine constants and P,T-parity nonconservation effects, which are described by the operators heavily concentrated in atomic cores, usually require accurate accounting for relativistic and correlation effects. However, precise all-electron four-component treatment of molecules and clusters with heavy elements is yet rather consuming. In turn, the relativistic effective core potential (RECP) calculations of valence (spectroscopic, chemical etc.) properties of such molecules are very efficient because the two-component RECP method allows one to reduce dramatically the computational cost providing a good accuracy of correlation and relativistic treatment for the valence electrons. However, the valence molecular spinors are usually smoothed in atomic cores and, as a result, direct calculation of electronic densities near heavy nuclei is impossible. The former circumstance stimulated further development of the RECP approaches and, in particular, the generalized RECP concept was developed [2] exploiting the idea of different treatment of inner core, outer core and valence shells. The latter had led to the methods of *nonvariational and variational one-center restoration* of correct shapes for four-component spinors in atomic cores after a two-component RECP calculation of a molecule [2]. In the report, the RECP and restoration methods are discussed. Their efficiency is illustrated in benchmark to-date correlation calculations of hyperfine structure and P,T-parity nonconservation effects in polar molecules YbF, PbO [2], HfF^+ [3], and liquid Xe [4] etc., which are of particular interest for the experiments on search for a new physics beyond the Standard Model.

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Calculation of electronic g-matrices of actinide compounds

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The molecular g-factors are crucial parameters in Electron Paramagnetic Resonance (EPR) spectroscopy. They parametrize the Zeeman effect that involves the interaction of a spin magnetic moment with a magnetic field. Before the 90's, g-factors were mostly calculated by semi-empirical methods while in the last decade, ab initio techniques have been developed based on wave functions or density functional theories either using a sum over states (SOS) expansion or using response theory [1]. We have recently proposed an alternative method based on wave function theory including spin-orbit effects by the SO-RASSI method [2]. This method has been applied with success to small molecules containing atoms until the third series of the transition metals and to a mixed-valence bimetallic complex [3] and the aim of this work is to applied it to actinide complexes. To our knowledge, only few attempts have been made to calculate g-factors of actinide complexes from first principles [4,5]. Relativistic effects in actinide complexes are important, so the deviation of g-factors from the value of the free electron is large and g-factors can even become negative. Most of the experiments measuring magnetic properties of actinide complexes date from the sixties. EPR and magnetic susceptibilities give the absolute values of the g-factors while experiment using ciculary polarized light provide the sign of the product of the three factors. Magnetic properties of these compounds are easily understood using ligand field theory models.

In this presentation, we first point out the arbitrary character of the g-matrix and specially discuss its transformation under a rotation in the spin space and we show that only the G tensor $gg^\dagger$ has a physical significance. Calculations first concern complexes with $5f^1$ configuration like the AnX_6^{q-}series with An = Pa,U,Np and X = F,Cl,Br and the NpO_2^{2+} cation either in the gas phase or with equatorial ligands. For the latter, the influence of the nature on magnetic properties of the equatorial ligands is discussed. Finally, the magnetic properties of Np^{4+} in Cs_2ZrCl_6 crystal are calculated. The ground state is in this case orbitally degenerate and cubic terms have to be added to the spin Hamiltonian. Both the linear term, namely the g-factor, and cubic terms are deduced from our calculations and compared to experimental values.

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A DFT Study of Acidity of Ortho- and Para-Substituted Aromatic Acids Using Molecular Descriptors

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Quantum chemical computations with full geometry optimization at the B3LYP/6-31G(d) level in aqueous phase at 298K are performed to calculate a set of molecular properties for 53 aromatic organic acids like benzoic acid, phenol, phenylacetic acid, cinnnamic acid, benzohydroxamic acid, benzenesulfonic acid, anilinium ion and their meta- and para-substituted derivatives. Molecular descriptors like ionization potential, electron affinity, hardness, chemical potential, global electrophilicity and free energy of deprotonation of these acids are computed. The local descriptors like Fukui functions and group philicity (Wg+) are calculated with MPA and HPA schemes. These aromatic acids are reacted with a strong base, OH-. The computed Gibbs free energy of deprotonation, the fractional numbers of electrons transferred,DeltaN and electrophilicity based charge transfer index, electrophilicity based charge transfer index (ECT) in acid-base reaction with a strong base, OH- and Wg+ are correlated with the experimental pKa values of these acids. It is found that this approach is particularly effective in discussing trends of changes in acidity of intimately related molecules. The effect of substituent on these descriptors is also studied. These parameters are correlated with experimental Hammett substituent constants (sigma). ECT and fractional number of electron transfer (DelN) correlate strongly with pKa and ? in separate groups of aromatic acids. Minimum energy, maximum hardness and minimum electrophilicity principles are tested for the acid-base reactions.

Key Words: Aromatic acids, Gibbs free energy, Hammett substituent constant, electron transfer, Electrophilicity based charge transfer index.

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Critique and Correction of Conceptual DFT

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Conceptual DFT (CDFT) and its applications have been the object of about one thousand research papers [1, 2]. CDFT assumes that the energy, E, is a continuous and differentiable function, E(N), of the number of electrons, N. The chemical potential, μ, and the chemical hardness, η, are defined as the first, and second partial derivatives of E(N) with respect to N. The chemical potentials of two systems, X and Y, are equalized as the systems start interacting. The CDFT electrophilicity index, ω, has found wide application [3-5].

A closer scrutiny of the foundations and applications of CDFT reveals, however, that it leads to severe contradictions to chemical principles and reality:

(i) The variation principle is violated; the CDFT equalization of μ lowers the energy of separated systems at large distances much below that of the isolated systems.

(ii) The charge transfer between X and Y is too small by a factor two. For the classical case of one-electron transfer at no cost, i. e., I(X)=A(Y) the equalization of μ is achieved by transfering just 0.50 electronic charge. Even for ionic diatoms, e. g., CsCl, the CDFT partial charge is below 0.50. Thus CDFT dipole moments are systematically too small.

(iii) According to the CDFT electrophilicity index the maximum uptake of electrons by any atom or molecule is smaller than one [3, 4], unless $A \geq I/3$. Stable anions are practically not existing according to CDFT.

The problems and contradictions are traced back to the occurance of spurious electron-electron attraction in case of fractional charges on the subsystems, X and Y [4, 6, 7]. Recent progress in properly incorporating the chemical context [7, 8] is reported. A different parabolic function E(N) for a defined chemical context, i. e., bond formation, accounts for the shared-pair aspects in charge transfer processes within chemical bonding. All of the above contradictions are resolved in this context, and very sensible results are obtained [4, 6, 7]. A generalized Born-Haber cycle with a common asymptotic reference energy for less polar solids and diatomic molecules is presented [7].

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A Linear-Scaling AO-Based MP2 Method for Large Molecules by Rigorous Integral Estimates

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Describing electron correlation effects for large molecules is a major challenge for quantum chemistry due to the strong increase of the computational effort with molecular size. In order to overcome this limitation, we present a rigorous method based on an AO-formulation of MP2 theory [1], which allows to avoid the conventional fifth-power scaling of MO-MP2 theory and to reduce the scaling to linear without loss of accuracy. The key feature of our method are multipole-based integral estimates (MBIE) [2,3], which account for the 1/R coupling in two-electron integrals and allow to rigorously preselect integral products in AO-MP2 theory. Here, the magnitude of products decays at least with $\frac{1}{R^4}$, so that a linear-scaling behavior can be achieved by numerical thresholding without sacrificing accuracy. The linear-scaling increase of the computational effort is reached much earlier than for HF or DFT approaches: e.g. the exact behavior of products indicates a scaling of $N^{1.0}$ from one to two DNA base-pairs for a 6-31G* basis. The number of significant elements in the pseudo-density matrices and of shell pairs hints to a very similar linear-scaling behavior for larger basis sets studied up to cc-pVQZ. First results of a preliminary implementation [4] show that an early crossover to conventional MP2 schemes for systems smaller than two DNA base pairs is observed, while already for a system with four DNA base pairs wins are at least a factor of 16 and the same accuracy is provided. Due to the linear-scaling behavior, these wins increase dramatically with system size.

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Excitation energy transfer rates from correlated transition densities

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Excitation energy transfer (EET) takes place if an electronically excited donor molecule decays to its ground state by simultaneous excitation of a neighbouring acceptor molecule. The process is of ultimate importance for the photophysical properties of e.g. biochemical systems or polymers and the distinct $1/R^6$ distance dependence of the leading dipole-dipole contribution to the EET rate (Förster Theory [1]) is widely applied for distance measurements on the nanometer scale. One approach to the calculation of the electronic contributions to EET coupling originates from symmetry-adapted perturbation theory and requires the knowledge of the transition densities of the monomers only. Owing to the size of the involved molecules, the vast majority of such investigations were carried out with semi-empirical models [2], however, more recently, transition densities from time-dependent density functional theory (TDDFT) have been employed as well [3].

Here, we report an implementation of the EET coupling matrix elements which accepts one-particle transition densities from arbitrary methods, ranging from configuration interaction with singly excited determinants (CIS) and the random phase approximation (RPA) to coupled-cluster theory. Particular interest is paid to a special coupled-cluster model, RI-CC2 [4], which is well suited to the treatment of fairly large chromophores.

For coupled-cluster methods, however, some surprising inconsistencies arise when comparing EET rates from the perturbational approach to those obtained from supermolecular calculations. These problems can be traced back to an incorrect separability of the two-particle transition density matrix which will be discussed in some detail. For the long-range interaction regime, it will be argued that results from the perturbational approach are superior to supermolecular calculations.

As an application, we discuss the EET rates in rylene-dyads, which have been previously studied by single molecule spectroscopy [5]. The questions in focus are (a) the role of bridge-assisted energy transfer and (b) the validity of Förster-theory for dyes with extended chromophores.

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Tubular aggregates of cyclic oligothiophenes. A theoretical Study

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Creation of hollow tubular structures by noncovalent self- assembly of appropriately crafted organic molecules has been the subject of considerable research in recent years [1]. Well-defined pi-conjugated macrocycles are of interest as modular building blocks for the assembly of new materials [2] and supramolecular architectures. Due to their toroidal structure, they could represent molecular circuits which would additionally include sites for recognition and selective complexation. In this respect, it is necessary to mention recently synthesized fully conjugated macrocyclic structures: cyclo(oligothiophene-diacetylenes)and cyclo[n]thiophenes [3]. capable of self-assembling. We have recently reported a theoretical study of oligothiophene catenanes and knots in different oxidation states [4] showing that the electronic properties of conjugated molecules depends in great extent on supramolecular architecture. The goal of this contribution is to study the effect of tubular aggregations of cyclic oligothiophenes on their electronic properties. The geometries of neutral, mono- and diionized cyclo[8]thiophene and the corresponding tubular aggregates containing 2,3,4 and 5 cyclo[8]thiophene units were fully optimized at MPWB1K level of theory using 3-21G* basis set. Closed and opened shell systems were calculated using RHF and UHF methods, respectively. Recently defined MPWB1K functional performs very well for non-bonding interactions which are of primary importance for tubular assembling of cyclooligothiophenes. Additional calculations carried out on cyclo[4]thiophene dimer showed that MPWB1K and MP2 models gave very similar geometries, while other popular functionals such as B3LYP and PBE0 strongly underestimate pi-pi stacking energies between thiophene fragments predicting significantly larger distances between cyclo[4]thiophene units in dimer compared to MP2 and MPWB1K models. It was found that binding energies between cyclo[8]thiophene macrocycles vary from 44.6 kcal/mol for dimer to 42.7 kcal/mol for pentamer in case of neutral aggregates. In case of monoionized species the binding energy increases (50.8 for dimer and 47.0 kcal/mol for pentamer) reflecting additional stabilization of positive charge by neighbour macrocycles. On the other hand, in case of dications the binding energy drops to 11.1 kcal/mol for dimer, further increasing to 42.8 kcal/mol for pentamer due to electrostatic repulsion. Calculations show that the most stable dicationic state for tubular aggregates is open-shell singlet. The energy difference between triplet and singlet states decreases with the number of units in tubular aggregates reflecting dissociation of a bipolaron into two separated polarons. This conclusion is also confirmed by the charge distribution analysis for charged tubular aggregates; In case of pentamer cation-radical the most of the positive charge is located at the middle macrocyle, while in case of dications the first and the last macrocycles are the most positively charged ones. The band gap estimation carried out at TD-B3LYP/6-31G* level reveals that even for pentamer (2.49 eV) it close to that found for isolated monomer (2.60 eV) rendering them as semiconductors. In conclusion tubular aggregates of cyclic oligothiophenes are stable formations with significant binding energy between macrocycles. They can be oxidized similar to linear polythiophene producing stable mono and dicationic species rendering them as attractive synthetic target for supramolecular chemistry.

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The Effect of Structural Parameters on the Polarizabilities of Methanol Clusters: A Hirshfeld Study

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Solvents form an interesting and challenging topic, which has been widely studied in the literature in the past decades. Although much progress has been already made in this field, many questions still remain in particular concerning the effect of solvents on the structures and properties of solutes. In order to try and understand those effects, one can start by investigating the structure and properties of the pure liquids, where single molecules can be regarded as a solute, surrounded by identical solvent molecules. In this study the dynamic structure of a liquid is approximated by the structure of clusters.

Although the structure of a single molecule in a cluster is simple to obtain, the knowledge of its properties usualy requires a partitioning method, of which the Hirshfeld method [1] is our method of choice. The Hirshfeld method was introduced in 1977 primarily as a method for the partitioning of charge density. Later it was extended for the partitioning of properties such as dipole moments, quadrupole moments, polarizabilities, energies and and others. Recently, Bultinck et. al. [2] have revised this method and proposed an iterative version, Hirshfeld-I, which is more in line with information theory.

The Hirshfeld-I method was used in this study for the analysis of polarizabilities of methanol clusters. The choice of the polarizability as the first property to be investigated is made because of its importance in the solvation process. The polarizabilities of fifty different methanol clusters, with aggregation numbers ranging between 2 and 12, were investigated. In a previous study on water clusters [3], the polarizabilities of water molecules in water clusters were found to be strongly and straightforwardly dependend upon the hydrogen bond network. The introduction of a methyl group into the structure of the molecule creates a more complicated system. Whereas the water molecule is a symmetric entity, which can form up to four hydrogen bonds when placed in a cluster (DDAA), the methanol molecule can only form three hydrogen bonds (DAA), due to the replacement of one hydrophilic part (OH) by an hydrophobic part (methyl group). Whereas the polarizabilities of the hydroxyl groups follow the trends established in the water clusters, the polarizabilities of the methyl groups exhibit a strongly different behaviour. The hydrogen bonding network as well as the polarizabilities are stronly affected by structural and sterical factors. The methyl groups were found to be especially sensitive to these effects. Finally, the influence of BSSE was studied by means of the counterpoise method and was found to be significant, increasing the polarizabilities of the water molecules by upto 10 percent.

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Proton transport in liquid phosphonic acid and polyphosphonic acid based polymers studied with molecular-dynamics simulations

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Polyphosphonic acids are promising candidates as proton conductors in proton-exchange membrane fuel cells. However, the proton conduction mechanism in these systems is only poorly understood. Atomistic molecular-dynamics (MD) simulations can considerably contribute to the understanding of the conduction process and the transfer mechanisms [1].

Currently, we are focussing on the proton transfer in liquid phosphonic acid and in model polymer structures. Therefore, we utilize density-functional based MD simulations [2]. For the liquid phosphonic acid we analyze the speed of the proton transfer (hopping rates), pair-distribution functions, diffusion coefficients, and geometrical conditions for the transfer. The influence of an excess charge carrier is also studied.
Using the results obtained from the simulations of the liquid, we simulate model polymer structures, e.g. poly-vinyl phosphonic acid. Here we can study the proton transfers along and between polymer chains varying their distance and relative arrangement. The role of additional water molecules is studied in both cases.

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Explicitly time-dependent configuration interaction simulations: Dipole switching in large molecules

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We report laser-driven charge transfer simulations for Li-(Ph)$_n$-CN ($n = 1, 2, 3$) using the TD-CIS (Time-Dependent Configuration Interaction Singles)[1] approach. These molecules are used as systematically extendable model systems, in order to investigate the selectivity, and thus controllability, of an ultra-short laser-induced electronic excitation as a function of the molecular size. For example, such control may be needed if a small electronic molecular switch is embedded in a larger molecular device.
We employ ultra-short π-pulses in order to induce an electronic excitation, *i.e.* a charge transfer transition, using the TD-CIS method within the fixed nuclei approximation[2,3]. The focus of our dynamical calculations lies on the selectivity of these π-pulses depending on their temporal width, and the molecular size. We show that for pulse widths larger than 1000 $\hbar/E_h$ the selectivity is lost mainly due to multi-photon transitions and dynamic polarizations of the molecules. For the latter processes a systematic dependence on the molecular size is observed, *i.e.* they get more important for larger molecules. Therefore, we believe that special care should be taken when simulating electronic transitions in extended molecular systems to include effects due to linear and non-linear polarizabilities. For large molecules and/or short and intense laser pulses few state models might actually overestimate the selectivity of laser excitations.

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Laser induced femtosecond dynamics in the excited states of β-carotene

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We present a three dimensional three state model for the theoretical description of the laser induced quantum dynamics, based on experimental, quantum-chemical and -dynamical data of β-carotene. From the electronic ground state the system is excited by a femtosecond pulse into the optically allowed S_2 state. Internal conversion to the vibrationally hot S_1 state via conical intersections is performed in about 180 fs. Here during 700 fs the system cooles down. The three state model was fitted to data of control experiments performed on β-carotene in the group of M. Motzkus. Here the internal conversion was followed by transient detection of the Raman active C-C and C=C stretch modes. Quantum chemical ab initio calculations were performed to specify the kinetic Hamiltonian, the Raman modes involved, their force constants and the relative position of the interacting potentials. With this model the mechanism of internal conversion is studied, incoorporating vibrational cooling in the S_1 state. The results are used to investigate the controllability of the transfer rate by modulated laser pulses.

A Monte Carlo - DFT study: Adsorption of organosilanes on polar ZnO (0001) surfaces

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The ultimate aim of the project is to investigate the mechanism of organosilane adsorption on zinc oxide surfaces using computational tools and various experimental techniques. The study of the processes during adsorption requires the selection of a proper model system to describe single molecule - surface interactions and to reveal the binding mechanisms.

In this study, polar ZnO (0001) surface is selected as the model substrate due to its abundance in amorphous zinc oxide. The main challenge in modeling of ZnO (0001) surfaces is the determination of the stabilization mechanisms to cancel the dipole moment between Zn and O terminated surfaces. Surface reconstructions, adsorption of OH^- on the Zn terminated surface and use of pseudo-oxygen atoms with 6.5 valency at the O terminated surface have been tested using SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) code. The binding energies of a variety of molecules to clean, hydroxylated and reconstructed surfaces have been computed to determine the most favorable binding state.

For the verification of computed binding energies, a Monte Carlo program[1,2] is developed that uses the binding energies calculated with SIESTA as input and produces the Thermo-Desorption Spectra. The comparison of different ZnO (0001) surface stabilization mechanisms, and the results of TPD experiments along with the Monte Carlo analysis will be discussed in the presentation.

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DFT study of ethylene dimerization by mixed bidentate P-N nickel complexes

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Short chain length α-olefins are strategic targets in industrial chemistry. Among the nickel(II) catalysts for ethylene dimerisation [1], the mixed bidentate P-N nickel complexes present some remarkable advantages [2]. In particular, the simplicity of their synthesis [3] and their excellent activity constitute strong arguments to deepen the explanation of the dimerisation process. Therefore a DFT study of the mechanism seems a crucial step to achieve a more precise understanding of the reaction process and to develop new catalytic systems.

Two mechanisms are investigated for three asymmetric model systems with various hindrances. The first one is the Cossee mechanism, previously studied for symmetric diimine nickel complexes by Musaev and al. [3]. The second one is the metallacycle mechanism that was proposed thirty years ago by Grubbs for monodentate nickel(0) complexes [4].

It was found that butene is always predominant for both mechanisms and that the elimination barrier is almost independent of the substituents on the nitrogen atom. On the contrary, the whole insertion process is all the more disfavoured as hindrance increases. The third insertion is actually the sum of two steps: the insertion itself and also the previous coordination of ethylene. In the hypothesis of a Cossee mechanism, this coordination occurs on the most destabilizing side (in trans of the phosphorus atom). This trans effect was linked with the increase of the Ni-N bond length. Moreover, the evolution of the NPPC dihedral angle suggests that the selectivity is all the best as the plane conformation of the ligand is more stabilized.

Finally, none definitive argument has been found to distinguish between both mechanisms, but several ways of improving the catalysts efficiency are deduced from the calculations.

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Nonadiabatic Coupling Mechanism for Ultrafast Electron Transfer in the Reaction Center of Bacterial Photosynthesis

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We investigate ultrafast electron transfer as a transition between adiabatic Born-Oppenheimer states which include the mixing of donor and acceptor orbitals

$$\phi_i = (c\phi_D + s\phi_A) \rightarrow \phi_f = (-s\phi_D + c\phi_A)$$

where the mixing coefficients depend on the energy gap ΔE and the resonance integral J .

$$cs = \frac{J}{\sqrt{\Delta E^2 + 4J^2}}$$

Within the harmonic parallel mode approximation the nonadiabatic matrix element for a transition involving creation of one quantum of the promoting mode s reads

$$V_{nad,s} = FCF \frac{1}{2Q_{s,0}} \int \phi_i(r;R) \bigtriangledown_{Q_s} \phi_f(r;R) dr$$

The Franck-Condon factor of the accepting modes was calculated for model systems of Bacteriochlorophyll and Bacteriopheophytine molecules on the basis of 6-31G/HF calculations. The electronic factor was evaluated with the help of the commutator relation $[\bigtriangledown_R, H] = \Delta E \partial V_{pot}/\partial R$ as

$$V_{nad,s} = FCF \quad \int \phi_i(r;R) \left(Q_{s,0} \bigtriangledown_{Q_s} V_{pot}\right) \phi_f(r;R) dr$$

and the potential energy was approximated by the Coulombic interaction with atomic point charges. Within these approximations the electronic factor was evaluated for the model systems on the 6-31G/HF basis by calculating all necessary two- and three center integrals. We found an almost continuous distribution of accepting and promoting modes. Our estimate of the transfer rate on the basis of the nonadiabatic coupling is much larger than the estimate by the conventional Marcus expression for the same values of the resonance integral J and the Franck-Condon factor giving time constants in the picosecond region even for resonance integrals as small as $10cm^{-1}$. The nonadiabatic coupling can be visualized as a dipole-dipole type interaction where the infrared dipole of the promoting mode is coupled to the transition dipole of the electronic transition, which is essentially given by cs times the change of the permanent dipole moment. A similar treatment was recently presented for ultrafast internal conversion processes during electron solvation [1].

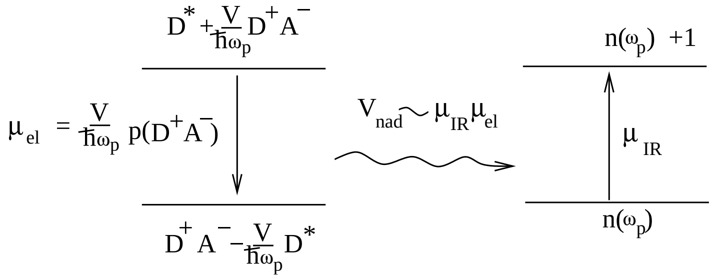

figure1: nonadiabatic dipole-dipole coupling mechanism

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Accurate computation of vibrational spectra for extended systems

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The prediction of accurate vibrational spectra from *ab initio* data has always been a challenging task in computational chemistry. One of the most promising methodologies to date that can simulate the vibrations of molecular systems of more than a handful of atoms is the vibrational self-consistent field technique and its extensions, combined with powerful parallelised quantum chemistry programs. This type of approach is very accurate, but the advantage of accuracy is often negated by the heavy demand on computational time. For this reason, the harmonic approximation has so far prevailed for most computational simulations of experimental vibrational data of large systems. In order to bring larger molecules within the reach of the self-consistent field techniques, we have developed over the past few years a new methodology for performing fast correlation-corrected vibrational self-consistent field (CC-VSCF or VCI) calculations using *ab initio* potential energy points generated on demand. This new method is based on an efficient reduction in the number of normal modes pair-coupling elements used in the CC-VSCF and VCI procedure. This approach saves computational time by focussing on the dynamically relevant part of the potential energy surface and neglecting the unused parts, leading to significant speedups compared to the usual VSCF approach, without significant loss of accuracy [1,2]. I will present our latest methodological developments and show applications of this new technique to achieve large speed improvements over the usual *ab initio* post-VSCF calculations

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Correlated bands in oxides with wave-function based methods

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We apply wave-function based quantum chemical methods to the study of electron correlation effects on the band structure of oxide compounds. Our analysis is based on a local Hamiltonian approach and performed on finite fragments cut from the infinite solid. As a first example we choose MgO, a relatively simple, weakly correlated ionic system. Localized Wannier functions and embedding potentials are obtained from prior periodic Hartree-Fock (HF) calculations. We investigate the role of various correlation effects in reducing the HF gap and modifying the band widths. On-site and nearest-neighbor charge relaxation as well as long-range polarization effects are calculated. Whereas correlations are essential for computing accurate band gaps, we found that in MgO they produce relatively small changes on the HF band widths. Our results [1] are in good agreement with the data derived from thermoreflectance and photoemission measurements. As a second example, we discuss the electronic structure of the copper oxide superconductors. We focus on the role of the underlying antiferromagnetic lattice in renormalizing the effective quasiparticle hoppings. Such effects are not accessible by standard density-functional calculations. In particular, the nearest-neighbor effective hoppings are reduced by a factor of 4 [2]. We show that the dispersion of the lowest bands observed in photoemission is reproduced with quantitative accuracy [2,3]. Additionally, the evolution of the Fermi surface with doping, from small hole pockets in the deeply underdoped region to a holelike shape with a pseudogap at intermediate dopings and an electronlike appearance in the overdoped regime, follows directly from our *ab initio* data. Our results thus open a new avenue for the first-principles investigation of the electronic structure of strongly correlated transition-metal oxides.

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Nanosized Metal and Oxide Particles as Realistic Models of Catalytic Materials

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It is now well recognized that the difference in complexity between single crystal surfaces and "real" catalysts cannot be easily bridged. This is one of the major obstacles, known as material gap in heterogeneous catalysis, which notably hinders the extension of profoundly understood processes on single crystal surfaces to equally good understanding of heterogeneous catalysis. Indeed, active components of working heterogeneous catalysts are commonly present in the form of rather large nanoparticles, exposing a variety of point and extended defects that in many cases determine the reactivity. Thus, for realistic modeling of such systems one should go beyond the single crystal description, which, however, continues to be very useful reference. To this end, so- called model catalysts in the form of well-characterized metal nanoparticles supported on ordered oxide films have been proven experimentally very fruitful [1]. The presentation describes our modeling strategy [2], developed to computationally represent at a sufficiently realistic level oxide-supported nanoparticles with 10**3 metal atoms, which are experimentally explored as model catalysts. This novel approach employs ordered three- dimensional nanoparticles of 10**2 atoms with structures cut from bulk and terminated by low-index surfaces; in this size range cluster properties are scalable to the bulk. Our density functional calculations of clusters from Pd55 to Pd146 showed that starting from 80 atomic particles the adsorption properties no longer exhibit size effects [2]. Thus, these models enable a realistic description of adsorption properties and reactivity of notably larger metal particles of similar shape in supported model catalysts [3]. Later applications of this modeling approach deal with structure of bimetallic PdZn particles containing 140 atoms and interactions with them [4], surface [5] and subsurface [6] impurities of light element atoms as well as reactions of methoxide (CH3O) decomposition on Pd nanoparticles [7]. Very recently, formation of arrays (nanowires) from Pd nanoparticles by self-assembling has been investigated [8] and extension of the modeling approach to metal-oxide particles of 200 atoms or more has been performed [9]. Examples of the above mentioned density functional applications of the nanoparticle modeling approach will be presented.

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Simulation of Photoluminescence Spectra of Neutral and Charged Exciton States in Self–Assembled Semi–Conductor Quantum Dot Molecules

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Semiconductor quantum dots (QDs) have attracted much interest since Qubits formed from interband charge excitations (excitons) represent a particularly promising system for quantum computation that can be coherently manipulated using picosecond laser pulses. An important step is to achieve coherent coupling of quantum states in spatially separated QDs to realize a system with conditional coherent dynamics that can be electrically and optically manipulated. In recent experiments on vertically stacked self assembled InGaAs/GaAs QD–molecules (QDMs) control of the coherent coupling between excitonic states in the upper and lower dots was achieved by tuning the electric field oriented along the axis of the QDM. Single molecule spectroscopy revealed a clear anticrossing of spatially direct (e, h in the upper dot) and indirect (e, h in different dots) single exciton states. Good accord was obtained with realistic calculations of the single exciton spectrum of the QDM, confirming that the tunnel coupling is mediated principally by the electron component of the exciton wavefunction.[1]

More recently the influence of electrostatically introducing an additional electron into the QDM was studied. This leads to the formation of negatively charged Trions for which the spectrum of anti–crossings reflects the complex interplay between Coulomb couplings and the electrostatic energies of the two dots. Trion states in QDMs can be either spatially direct (e.g. $2e + 1h$ in upper dot) or indirect (e.g. $1e + 1h$ in upper dot and $1e$ in lower dot) and can be tuned into resonance by tuning the static electric fields. Furthermore, radiative decay takes place to a $1e$ final state that, itself, can hybridize over the two dots. Each anticrossing ($1e+1h$, $2e+1h$ initial and $1e$ final states) occurs at a distinct field, allowing for their clear identification. The richness

of the spectra is further enhanced by spin–spin effects whereby singlet and triplet Trion states exhibit remarkably different behavior.
A simple model describing all possible spin–adapted many–particle states in the effective mass approximation yields a detailed analysis of the spectra. The excellent agreement with the experiment allows us to assign all observed features with confidence.[2]

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Laser-controlled chiral molecular switch: Quantum simulations for the stereoselective transformation between achiral and chiral atropisomers

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The influence of molecular chirality on the outcome of chemical or biochemical processes is still an important topic of today's research. For instance, reaching perfect control of the stereoselectivity in a chemical reaction remains one of the great challenges in chemistry. Traditional chemistry offers a variety of effective and well-established methods for stereoselective synthesis, e.g. by employing a chiral catalyst which drives the reaction towards the desired stereoisomer. In this case, a change of the handedness of the catalyst, e.g. induced by an external laser field, controls which stereoisomer is produced by the reaction. Indeed, chemical compounds, so-called chiroptical switches, exists that undergo isomerization upon irradiation at the appropriate wavelength resulting in a change of the chirality of the system [1]. In addition, various applications of chiroptical switches are possible in the field of nanoscale devices ranging from liquid crystal displays to data storage and information processing [2].
We report model simulations for a laser-operated chiral molecular switch, namely 1-(2-cis-fluoroethenyl)-2-fluorobenzene. This styrene derivative supports one achiral and two chiral atropisomers, the former being the most stable isomer at room temperature. In quantum wavepacket propagations the isomerization of 1-(2-cis-fluoroethenyl)-2-fluorobenzene is investigated based on electronic ground and excited state potentials obtained from (TD)DFT calculations. Using IR laser pulses the molecule is excited to an internal rotation around its chiral axis, i.e. around the C-C single bond between phenyl ring and ethenyl group, causing a change of the chirality. On the basis of stereoselective laser pulses [3], a laser control mechanism was developed which allows for the selective switching between the achiral and either the left- or right-handed form of the oriented molecule [4], see Fig. 1. To orient the molecule it is bonded to adamantane which on his part serves as rigid molecular tripod to be chemisorbed, e.g. on a gold surface via thiol linker groups [5]. The symmetry of the adsorbent defines the orientation of the molecule which influences the selectivity and efficiency of the control.

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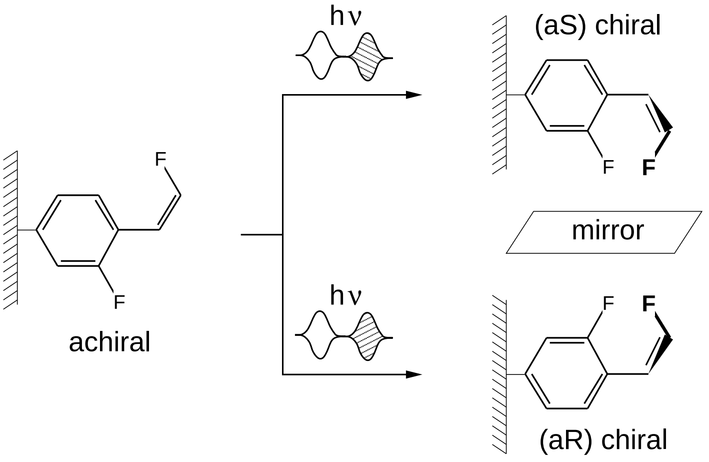

Figure 1: Stereoselective laser pulses control the transformation between the achiral and either left- or right-handed atropisomer of 1-(2-cis-fluoroethenyl)-2-fluorobenzene.

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Taming of a beast: Multi-mode nonadiabatic excited state dynamics in NO_3

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NO_3 is a D_{3h} symmetrical radical of considerable interest in atmospheric chemistry. Furthermore, it poses a number of tremendous challenges for its theoretical treatment, making it a very interesting benchmark system for method development.

The problems of obtaining accurate *ab initio* electronic structure data was solved only recently by large-scale MRCI calculations.[1] The ground and low-lying excited states can now be computed reliably and in excellent agreement with available experiments.[2] This methodology has been used to compute coupled full-dimensional potential energy surfaces (PESs) for the first excited state ($^2E''$). The *ab initio* data is represented by a diabatic potential matrix, accounting for the strong Jahn-Teller (JT) effect in the doubly degenerate excited state and also for mode-mode couplings between different vibrational coordinates. It turns out that higher-order JT couplings are important for a reasonable description of the complicated PESs. The necessary matrix elements were derived recently[3] and lead to excellent fitting results for the strongly anharmonic PESs.

The development of the surfaces enabled us to study the multi-mode nonadiabatic dynamics of the $^2E''$ state that follows photodetachment from NO_3^-. In a first study, only terms up to second order were retained in the potential matrix. Such a vibronic coupling approach is often sufficient to obtain very good spectra. However, the computed detachment spectrum, though in reasonable agreement with experiment, shows significant differences in the details.[4] In the present study higher-order JT and additional mode-mode couplings are included in the dynamics calculations. This leads to a significantly improved agreement with experiment, demonstrating the importance of mode-mode and higher-order couplings.

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Adsorption energy calculations with the method of increments: Application to the adsorption of CO on the CeO_2 110 surface

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Adsorption processes like CO on the CeO_2 110 surface contain two types of interactions: dispersion and classical electrostatics. Dispersion is a part of the electron correlation that is often referred to a long-range and non-local electron correlation. It is by definition not included in the Hartree-Fock (HF) formalism and is usually not incorporated in density functionals due to the local character of the functional as well. (DFT results are published in [1].) The classical electrostatic interaction between CO consists of the interactions of dipole, quadrupole and all higher moments of CO with the surface of ceria. To describe both effect on an equal footing, it is necessary to use highly accurate wavefunction-based correlation methods like the coupled cluster approach.

But a full CCSD(T) treatment of all atoms which are involved in the binding is not feasible with nowadays computers. Therefore the method of increments is used for the problem. Originally it was invented to calculate the correlation energy of extended systems in terms of contributions of localized orbital groups (for a review see [2]). Here for the first time the method of increments is applied to the adsorption of molecules on surfaces. The main idea is an expansion of the correlation energy of the joint system (surface and adsorbate) in terms of correlation contributions of localized orbital groups numbered $i, j, k, ...$

$$E_{\text{corr}} = \sum_i \epsilon_i + \frac{1}{2}\sum_{\substack{ij\\ i\neq j}} \Delta\epsilon_{ij} + \frac{1}{6}\sum_{\substack{ijk\\ i\neq j\neq k}} \Delta\epsilon_{ijk} + \cdots . \qquad (1)$$

One group will be the localized orbitals from the adsorbed molecule, the other groups will be the individual atoms in the solid. We have to take as many into account as their correlation contribution is changed due to the adsorbtion process. We calculate the adsorption energy at the CCSD(T) level with the method of increments and compare to MP2 results, which can be performed both within the incremental expansion and within a full correlation calculation.

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Bonding Properties in Elemental Zn and Cd

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The structures of intermetallic phases are not only governed by the number of valence electrons but also by their degree of localization and the transfer of electrons between the constituents. As a consequence, structures can considerably deviate from close packing, a fact that is not yet understood, even for metallic elements like Zn and Cd, which stick out from the hexagonal close packed elements due to the exceptionally large c/a ratio.

The studies presented here combine theoretical and experimental investigations to determine the electronic structure of Zn and Cd in position and in momentum space in comparison to that of Mg, which has formally the same valence electron configuration, but in contrast to Zn and Cd, a nearly ideal c/a ratio.

DFT calculations were performed with various local and gradient corrected functionals including hybrid functionals [1]. Although the anisotropy of the bonding is not described in a well-balanced manner at this level of theory, the role of electronic correlation, involving also the filled d-shell, and the different nature of the intra- and inter-layer interactions can be obviously deduced from the results. The potential energy surface with respect to the lattice constants, PES(a,c), proved to be very flat along a path that corresponds to a uniaxial compression along the c axis. Depending on the method and the computational parameters, even a second local minimum is apparent. Although the band structure and the topology of the Fermi surface varies along this path, leading to a Mg-like appearance at the second minimum, these changes are not reflected in the computed difference electron densities and Compton profiles.

In order to get hints whether the special shape of the potential energy surfaces of Zn and Cd is an artefact of DFT or a real property of the elements, wave-funtion-based methods are applied, computing the correlation energy by means of the method of increments.[2,3] The viability of this approach for group II metals has been demonstrated.[4,5] Preliminary calculation for Zn indeed show a second minimum on PES(a,c), being however separated from the first one by a rather high barrier.

Both, the static deformation densities obtained from multipole refinement of the X-ray diffraction data, and the anisotropy of the measured Compton profiles look similar to the computed DFT-results. However the measured differences between Mg and Zn are more pronounced.

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Titles of posters

[The abstracts can be obtained upon request to the organizers (stc07@mx.uni-saarland.de).]

1. Explicitly Correlated Local MP2-Theory
   T.B. Adler,[1] G. Knizia,[1] O. Marchetti[1], F.R. Manby[2] and H.-J. Werner[1]
   [1] *Institut für Theoretische Chemie, Universität Stuttgart, Stuttgart, Germany*
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2. Theoretical and Spectroscopic Study on 2-Substituted 1,3-Indandiones as Potential Optical Sensors for Metal Ions
   Anife Ahmedova[1] and Michael Springborg[2]
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   [2] *Physical and Theoretical Chemistry, University of Saarland, Saarbruecken 66123, Germany*

3. Simulation study of the structure and dynamics of the Alzheimer's Amyloid beta (Abeta) peptide monomer in aqueous solution
   Priya Anand,[1,2] Ulrich. H.E. Hansmann,[1] and F.S.Nandel[2]
   [1] *John von Neumann Institute for Computing, Forschungszentrum Jülich, 52425 Jülich, Germany*
   [2] *Department of Biophysics, Panjab University, Chandigarh, India*

4. The total number of bound states in a given attractive potential
   V. Koch, D. Andrae
   Theoretische Chemie, Fakultät für Chemie, Universität Bielefeld, Bielefeld, Germany

5. Noncovalent Interactions between Graphene Sheets and in Multishell (Hyper)Fullerenes
   J. Antony,[1] C. Mück-Lichtenfeld,[1] and S. Grimme[1]
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6. Assessment of local hybrid functionals for thermochemistry and barriers
   H. Bahmann,[1] A.V. Arbuznikov,[1] and M. Kaupp[1]
   [1] *Institut für Anorganische Chemie, Julius-Maximilians-Universitt, Wrzburg, Germany*

7. Correlation factor model
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8. Hidden Dynamical Quasi-Symmetry in Optical Absorption and Ionization Spectra of Quantum Dot Nanorings
   I. Bâldea* and L. S. Cederbaum
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9. Decomposition of Methylamine (CH_3NH_2): Spectroscopy and Kinetics
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10. Vanadium Oxide Compounds with Quantum Monte Carlo
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11. Unbiased study of stochiometric $(CdS)_n$-Cluster
Michael Bauer,[1] Yi Dong,[1] and Michael Springborg,[1]
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12. Metadynamics Simulations of Phase Transitions in Silicon
Using a Novel High-Dimensional Neural Network Potential
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13. Probing the Photoswitch:
non-adiabatic Hybrid QM/MM MD Studies of Liquid Azobenzene
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14. Theoretical Study of Electrochemical and IR Spectroscopic Properties of
Transition Metal Coordinated Scorpionates
J. Borowka,[1] H. Vitze,[1] M. Wagner,[1] and M. C. Holthausen[1]
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J. Brandão[1] and C.J. Rosa[1]
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J. Brandão[1] and C.M.A. Rio[1]
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17. Molecular dynamics simulations of dendrimer-encapsulated α-Keggin ions in trichloromethane solution
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18. On the Chelate Effect in Uranyl Complexes

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19. Point defects in CeO_2 and CaF_2 investigated using the periodic fast multipole electrostatic embedding scheme

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20. Molecular Dynamics Simulations for a Light-Driven Molecular Motor

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21. MO-based prediction of rate constants for the indirect photolysis of organic compounds

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22. All-electron Douglas-Kroll-Hess and pseudopotential study on the low-lying states of Uranium hydride UH

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23. (s)-N-Acetylproline Amide in Liquid Water: Assessing the Quality of the Continuum Solvation Approach

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24. Metal-Ligand Mo-X (X = P, N, PO, and NO) Bond Situation in Mo Complexes

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25. Structural and electronic analysis of lanthanide complexes: *f* orbitals may be not just spectators and reactivity may not necessarily be independent of the identity of the lanthanide atom; a DFT study

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26. Assessment of the Exchange-Correlation Functionals for the Physical Description of Spin Transition Phenomena by DFT Methods: All the Same?
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27. Through-bond versus through-space contributions on excitation energy transfer in condensed phase
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28. ROKS simulation of the excited-state dynamics of pyrrole
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29. Molecular and Electronic Architecture of Bimetallic Anionic $[\textit{cyclo}\text{-}\mathrm{Cu_3Au_3}]^-$ Homotops
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30. Hybrid Density Functional Theory Study of Photoluminescence Spectra of Platinum II Porphine and Platinum II Octaethylporphine
    Cristian V. Diaconu,[1] Richard L. Martin,[1] Darryl L. Smith,[2] Enrique R. Batista,[1] Brian K. Crone,[3] Scott A. Crooker,[4] and Ian H. Campbell[3]
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31. Substituted Azobenzene Molecules as Molecular Switches: Quantum Chemical Investigations

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Yi Dong and Michael Springborg
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33. Decoherence Mechanisms in Nanotechnology
G. Doyen,[1] D. Drakova[2]
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34. The Role of Decoherence for STM induced CO desorption on Cu(111)
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35. Efficient Algebraic Evaluation of Second Quantized Operator Strings: Term Generation and Simplification
A. Engels-Putzka[1] and M. Hanrath[1]
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36. A Theoretical Investigation on the Influence of the Microhydration on the Vertical and Adiabatic Spectrum of 1-Methylthymine
M. Etinski[1] and T. Fleig[1]
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37. Multi-mode vibronic interactions in fluorinated benzene radical cations
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38. Direct Estimate of Conjugation, Hyperconjugation, and Aromaticity with the EDA Method.
I. Fernández and G. Frenking
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39. Ultrafast Dissociation Pathways of Diphenylmethyl Chloride to Generate
Reactive Carbo Cations
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40. Superexchange and double exchange in diluted magnetic semiconductors
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41. Ab-initio DFT/TDDFT study of manganese porphyrin systems
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42. Implementation of the Incremental Scheme and Application to CCSD Energies
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43. Implementation of the Incremental Scheme for CCSD Energies
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44. Solving ROKS equations in excited state molecular dynamics simulations
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45. First-Principles Calculations of Magnetic Circular Dichroism Spectra
Dmitry Ganyushin and Frank Neese
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46. Optimizing the DFTB repulsive energy using genetic algorithms
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47. ^{51}V NMR Chemical Shifts Calculated from QM/MM Models of Vanadium Chloroperoxidase
K.R. Geethalakshmi, M. Bühl, Mark P. Waller, Dongqi Wang, and Walter Thiel
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48. Understanding Enzymatic Reaction Mechanisms using QM/MM Simulations:
Hydrolysis of Nucleotides in Membrane-Bound hGBP1
R. Glaves, A. Chaumont, G. Mathias, and D. Marx
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49. Presence or absence of metal-metal bonding in boron- and carbon-bridged dinuclear transition metal complexes from ELF and AIM studies
K. Goetz, M. Kaupp
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50. Coupling of Short-Range Density Functional Theory With Long-Range Wavefunction-based Methods: New Results

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51. Binding of Uranyl(VI) and Pertechnetate Ions in Water
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52. Non-adiabatic dynamics on open shell systems: Application to OHF.
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53. Surface states on Xe covered Cu(111)
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54. Theoretical analysis of simple models of nitrogenases based on molybdenum (III). Modification of the electronic environment to modulate the catalytic activity
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55. Dynamic Protonation Equilibrium of Solvated Amino Acid Side Chain Analogues
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56. Quantum dynamics calculations of the ground state tunneling splitting
    in malonaldehyde
    Thorsten Hammer[1] and Uwe Manthe[1]
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57. Application of MRexpT:
    N_2 and LiF as higher excitations of H_4, P_4, BeH_2
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58. Investigation of some truncated Coupled Cluster Variants
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59. Reactions of Transition Metal Carbenes With Ethylene
R. Haunschild and G. Frenking
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60. Quantized density-functional theory for molecular fluids in nanoporous materials
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61. Restriction of Vibrational Coupling Contributions in Molecular Cluster Calculations
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62. Benchmarking the performance of spin-component scaled CC2
in ground and electronically excited states
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63. Efficient implementation of recent developments in MP2-F12 theory and its application to chemical problems
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64. Interaction of probe molecules with the metal organic framework (MOF) CPO-27-Ni examined by periodic DFT calculations
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65. Quantum chemical calculations on Ni_2O_2 and ${Ni_2O_2}^+$
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66. Vibronic Structure Methods for Larger Molecular Systems:
Theoretical Prediction on Photoelectron Spectra of RNA-Building Blocks
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67. Exploring the Photo-induced Green-to-Red conversion of Fluorescent Protein EosFP
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68. Molecular parity violation in open-shell systems
within a electroweak quasirelativistic approach

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69. Molecular Dynamics investigations on DJ-1 protein and its mutants associated with Parkinson's disease
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70. Dynamical and Static Models of n-Butylboronic Acid - Comparison with Experiment
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71. First principle molecular dynamics simulations of selected model structures of hydrogen-bonded Schiff and Mannich bases - comparison with experimental data
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72. Atomistic Modelling of Mechanical Properties of Silicon
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73. Unraveling the Effect of NH_3 co-Ligation on the Catalytic Efficiency of Fe^+ Ion in Gas Phase Carbon Dioxide Fixation Reactions
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74. Deposition of Ni_{13} and Cu_{13} clusters on Ni(111) and Cu(111) surfaces
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75. Transition strength and first-order properties of excited states from local CC2 for large molecules
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76. Tracing Photochemical Products of NBA by Resonance Raman Spectroscopy
    K. Kiewisch,[1] S. Laimgruber,[2] P. Gilch,[2] and J. Neugebauer[1]
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77. Parallelization of large-scale relativistic multi-reference configuration interaction programs with application to (RbBa)$^+$ and the thorium diatom
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78. Static electric dipole polarizabilities for closed shell atoms and ions
    V. Koch, D. Andrae
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79. Calculation of excitation energies employing the TPSS meta-GGA
    S. Kossmann and F. Neese
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80. Tuning the reactivity of ZnO(10$\bar{1}$0) surfaces by coadsorption of CO$_2$ and characterization of the adsorbate structures by STM data calculations
    R. Kovacik, B. Meyer, and D. Marx
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81. On the elliptic relation between physical and mathematical entanglement
    T. Krüger[1]
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    Institut für Chemie, Karl-Franzens-Universität Graz, 8010 Graz, Austria

82. Quantum-Chemical Study on the Effect of Lewis Acid Centers in a Poly(ethylene oxide)-Based Solid Electrolyte
    P. Kubisiak and A. Eilmes
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83. Second order Møller-Plesset treatment of molecular hydrogen
    physisorption on MOF-5
    A. Kuc,[1] G. Seifert,[1] T. Heine,[1] and H. Duarte,[2]

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84. Unbound exciton-phonon states in oligothiophene crystals – a model approach for spectroscopic purposes
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85. Application of *short-range*-DFT/ *long-range*-Coupled-Cluster method to Lanthanide Diatomics
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86. Open-Shell Local Coupled Cluster Theory
Y. Liu and H.-J. Werner
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87. Raman Optical Activity Spectra: Analysis of the Role of the
Electric-Dipole–Electric-Quadrupole Tensor
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88. 2,2'-Bipyridyl Ytterbocene Complexes: Molecular Kondo Singlet Analogs?
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89. The Density Matrix Renormalization Group Method Facing the Spin State Problem in Quantum Chemistry
K. H. Marti,[1] G. Moritz,[1] I. Malkin Ondik,[1] and M. Reiher[1]
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90. Analytic High-Order Douglas–Kroll–Hess Electric Field Gradients
R. Mastalerz,[1] G. Barone,[2] R. Lindh,[3] and M. Reiher [1]
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91. Ab initio study of hydrogen storage in MOFs
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92. DFT/Metadynamics Study of the Methanol Synthesis on ZnO Catalysts
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93. Simple Gaussian Model Density to Describe Electrostatic QM/Pot Interaction
F. Mohamed[1] and J. Sauer[1]
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94. Relativistic Energy-consistent 5f-in-core Pseudopotentials for Penta- and Hexavalent Actinides
A. Moritz[1] and M. Dolg[1]
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95. Towards the chemistry of element 112 (eka-mercury). Benchmark relativistic calculations of properties of E112 vs. Hg compounds.
N.S. Mosyagin,[1] A.V. Titov,[1] A.N. Petrov,[1] T.A. Isaev,[1] A.V. Zaitsevskii,[2] and E.A. Rykova[3]
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96. Parity Violating Nuclear Magnetic Resonance Parameters:
Scaling Laws and Conformational Effects
S. Nahrwold,[1] M. Bühl,[2] and R. Berger[1]
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97. Docking with PSO@Autodock: A Novel Fast Docking Program Employing the *var*CPSO-ls Particle Swarm Algorithm
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98. Methodological Developments in the Theory of the Zero-Field Splitting Tensor
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99. Photochemistry of nucleobases: An nonadiabatic *ab initio* molecular dynamics study of uracil in aqueous solution
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100. Molecular Magnetism: An *ab initio* study of a hexanuclear ferric wheel
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101. Hydrogen halides photochemistry on small water particles: Joint theoretical and experimental study

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102. Electrophilic Reactivity of Michael-Type Acceptors

Norbert Ost,[1] Alexander Böhme,[1] Ralf-Uwe Ebert,[1] Ralph Kühne,[1] Gerrit Schüürmann[1,2]

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103. Computational structural investigations of bilirubin binding motif analogues

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104. An unexpected requirement for the DFT treatment of agostic interactions: the uniform electron gas correlation limit.

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105. Theoretical studies of excitation energy transfer between two benzene molecules

J. Pfister,[1] R.F. Fink,[1] and B. Engels[1]

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106. Pigment Yellow 101: An example for the rich photochemistry of medium-sized molecules

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107. Joint theoretical and experimental study of the water/corundum (Al_2O_3) interface: An application to the safety assessment of nuclear waste disposal

R. Polly,[1,3] B. Schimmelpfennig,[1,3] M. Flörsheimer,[1,3] K. Kruse,[1,3] A. Abdelmonem,[1,3] R. Klenze,[1] and Th. Fanghänel[2]

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108. ^{31}P Chemical Shift Tensors in RNA and DNA Backbone. A DFT Study of Conformational Dependence and Its Implications for NMR Studies
J. Přecechtělová, P. Padrta, M.L. Munzarová and V. Sklenář
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109. Lagrangian approach to molecular vibrational Raman intensities
D. Rappoport[1] and F. Furche[1]
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110. Structures and energetics of pure and mixed acetylene-ammonia clusters
B. Real and G. Jansen
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111. Vibrational properties of adsorbates on surfaces
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112. A theoretical modeling of cysteamine solutions Raman spectra
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113. A String-Based Implementation of Explicitly-Correlated Coupled-Cluster Theory
Gareth W. Richings,[1] Wim Klopper,[2] and Andreas Köhn[1]
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114. Embedded Cluster calculation on the ZnO-Catalyzed Synthesis of Methanol from CO and H_2
G. Rossmüller,[1] V. Kleinschmidt,[1] and C. Hättig[1]
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115. HYLLERAAS-TYPE WAVE FUNCTIONS FOR ATOMS AND SMALL MOLECULES
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116. QM/MM Study of BlrB: a BLUF Domain Protein
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117. QM/MM Studies on Adsorption Compelxes in Zeolites
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118. A new method for correlated dynamics of many electron systems with reduced density matrices
B. Schäfer-Bung, M. Nest, and P. Saalfrank
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119. An improved algorithm for the calculation of non-expanded second-order exchange contributions in the framework of the combined density functional and symmetry-adapted perturbation theory approach
R. Schäffer, G. Jansen
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120. Phenol$(H_2O)_{1\leq n\leq 3}$ revisited: An *ab-initio* study on the photophysics at the level of Coupled Cluster response theory
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121. Representation of the eigenfunctions of $\hat{L}^2$ with one dimensional basis functions
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122. Joint theoretical and experimental research on actinide compounds
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123. Density-Functional Study of Electronic Structure and EPR Parameters of Biologically Relevant Manganese Complexes
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124. Rotational excitation and cross sections in the reaction $Cl^- + CH_3Br \rightarrow ClCH_3 + Br^-$
S. Schmatz and C. Hennig
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125. An anisotropic Heisenberg model on the trigonal lattice for multiferroic oxides
M. Schreiber,[1] T. Kunze,[1,2] C. Olbrich,[1,3] and S. Gemming[4]
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126. Improvement of trial wave functions for quantum Monte Carlo
A. Schwarz,[1] R. Berner,[1] and A. Lüchow[1]
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127. Gold Nanoparticles Without and With Ligands
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128. Prediction of Hydrogen Bond Donor and Acceptor Strengths of Organic Compounds
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129. Structures and energies of mono-sulphated dimers from carrageenans by DFT method
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130. Electronic structure of excited electronic states of tryptophan and N-acetyl tryptophan methyl amide (NATMA)
D. Shemesh and W. Domcke
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131. Are six isomers involved in folding if tryptophan
is one of the amino acids in the peptide?
D. Shemesh and E.W. Schlag
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132. Theoretical investigation of the heavy-atom analogues of acetylene E2X2 (E = Si-Pb, X=F-I)
Takayasu Shimizu and Gernot Frenking
Department of Chemistry, Philipps-University Marburg, Hans-Meerwein-Strasse, D-35032 Marburg, Germany

133. A Combined DFT and High Resolution 27Al NMR Study of Isolated Aluminum Atoms in the Framework of ZSM-5 Zeolite
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134. Quantumchemical studies of the adsorption of single acetone molecules on hexagonal (Ih) and cubic (Ic) ice polymorphs.
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135. How much can donor/acceptor-substitution change the responses of long push-pull systems to DC fields?
M. Springborg
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136. The extended Algebraic Diagrammatic Construction scheme of second order (ADC(2)-x) for Open-Shell Molecules: A Study of Polyene Cations and Polyenyl Radicals
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137. Many-Electron Bands in Transition Metal Compounds
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138. Implementation of a vector potential method in an *ab initio* Hartree-Fock program
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139. Monte Carlo Simulation of Temperature Programmed Desorption Including Binding Energies and Frequency Factors Derived by DFT Calculations
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140. A Refined Unsymmetric Lanczos Eigenvalues for Computing Accurate Eigentriplers of a Real Unsymmetric Matrix

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141. Theoretical Studies of homogeneous SiGe clusters and their comparison with pure Si and Ge clusters using Density Functional Tight binding (DFTB) method
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142. Moment-constrained two-step Density Fitting in periodic local MP2 (DFP-LMP2). Application to molecular crystals and adsorption on surfaces.
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143. Infrared Spectroscopy and Dynamics of the Protonated Water-Dimer
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144. Theoretical study of the C-H activation mechanisms with uranium(IV) and thorium(IV) bismethyl complexes
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145. A Comparative Study of Single Reference Correlation Methods of the Coupled-Pair Type
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146. Modeling Biological $\mathrm{U}^{\mathbf{VI}}$ Coordination from First Principles
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147. Theoretical study of adsorption of methanol and toluene on zeolite surfaces
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148. Equilibrium structures of the adenine thymine base pair
in the ground and first excited state
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149. Comparing Ring Polymer and Centroid molecular dynamics methods
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150. Transition States of the H Abstraction from Amines through Reaction with OH Radicals
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151. A Local Version of the Algebraic Diagrammatic Construction Scheme to Calculate Electronic Excited States of Large Molecules
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152. The dynamics of angular degrees of freedom: new basis set and grid representations of Hamiltonian operators
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153. Combination of Spectroscopy and Quantum Chemistry in Elucidating the Reaction Mechanisms of Nonheme Iron Enzymes
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154. Hydrogen storage in nanoporous materials
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155. Beyond the featureless particle approximation: An extension of quantum-liquid density-functional theory to account for rotational effects
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156. Theoretical Investigation of the Molecular Properties of Cerium Trichloride $CeCl_3$
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157. Theoretical estimation of Zero-Field Splitting Tensor
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158. STM-induced Switching of Hydrogen on a Silicon(100) Surface:
An Open-System Density Matrix Study
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159. *Ab initio* Calculation of Excitation Energy Transfer between two Perylene Bisimide Molecules
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160. Antitumor activity of a copper(II) chelate complex. An approach in the explanation of the mechanism of action through molecular modelling and docking studies
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161. Absorption Spectra Simulation for Small Donor-Acceptor Molecules with Density Functional Method
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162. Assessment of the High Accuracy Extrapolated Ab Initio Thermochemistry (HEAT) method for the computation of ionization potentials.
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163. α,$\delta-$Hybrid Peptides as Peptide Mimetics
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164. Analytical Gradients in a Subsystem Formulation of Density Functional Theory
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