

John von Neumann Institute for Computing (NIC)

Johannes Grotendorst (Editor)

Modern Methods and Algorithms of Quantum Chemistry

Winterschool, 21 - 25 February 2000

Forschungszentrum Jülich, Germany

Poster Presentations

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PREFACE

Computational quantum chemistry has long promised to become a major tool for the study of molecular properties and reaction mechanisms. The fundamental methods of quantum chemistry date back to the earliest days of quantum mechanics in the first decades of the twentieth century. However, widespread quantitative applications have only become common practice in recent times, primarily because of the explosive developments in computer hardware and the associated achievements in the design of new and improved theoretical methods and computational techniques. The significance of these advances in computational quantum chemistry is underlined by the 1998 chemistry Nobel prize to Walter Kohn and John Pople; this award also documents the increasing acceptance of computer simulations and scientific computing as an important research method in chemistry.

Nearly one third of the projects which use the supercomputing facilities provided by the John von Neumann Institute for Computing (NIC) pertain to the area of computational chemistry. For projects in quantum chemistry the Central Institute for Applied Mathematics (ZAM) which runs the Cray supercomputers and networks at the Research Centre Jülich offers several extensive software packages running on its supercomputer complex. The computational requirements of large quantum-chemical calculations are enormous. They have made the use of parallel computers indispensable and have led to the development of a broad range of advanced algorithms for these machines. The goal of this Winterschool is to bring together experts from the fields of quantum chemistry, computer science and applied mathematics in order to present recent methodological and computational advances to research students in the field of theoretical chemistry and their applications. The participants will also learn about recent software developments and about implementation issues that are encountered in quantum chemistry codes, particularly in the context of high-performance computing (topics not yet included in typical university courses). The emphasis of the Winterschool is on method development and algorithms, but state-of-the-art applications will also be demonstrated for illustration. The following topics are covered by twenty lectures:

- Density functional theory
- Ab initio molecular dynamics
- Post-Hartree-Fock methods
- Molecular properties
- Heavy-element chemistry
- Linear scaling approaches
- Semiempirical and hybrid methods
- Parallel programming models and tools
- Numerical techniques and automatic differentiation
- Industrial applications

The programme was compiled by Johannes Grotendorst (Forschungszentrum Jülich), Marius Lewerenz (Université Pierre et Marie Curie, Paris), Walter Thiel (MPI für Kohlenforschung, Mülheim an der Ruhr) and Hans-Joachim Werner (Universität Stuttgart).

Fostering education and training in important fields of scientific computing by symposia, workshops, schools and courses is a major objective of NIC. This Winterschool continues a series of workshops and conferences in the field of computational chemistry organized by the ZAM in the last years; it provides a forum for the scientific exchange between young research students and experts from different academic disciplines. The NIC Winterschool will host more than two hundred participants from sixteen countries, and more than fifty abstracts have been submitted for the poster session. This overwhelming international resonance clearly reflects the attractiveness of the programme. The excellent support of the Arbeitsgemeinschaft für Theoretische Chemie in preparing the Winterschool is highly appreciated.

As in previous conferences, many people have made significant contributions to the success of this Winterschool. The local organization at Research Centre Jülich was perfectly done by Elke Bielitz, Rüdiger Esser, Bernd Krah-Urban, Monika Marx, Renate Mengels, and Margarete Reiser. We are grateful for the generous financial support by the Federal Ministry for Education and Research (BMBF) and by the Research Centre Jülich and for the help provided by its Conference Service. We also thank the authors for their willingness to provide a written version of their lecture notes. Special thanks go to Monika Marx for her commitment concerning the composition and realization of the proceedings and the book of abstracts of the poster session. Finally, we are indebted to Beate Herrmann who supported the typesetting of these books with professionalism and great care.

Jülich
February 2000

Johannes Grotendorst

Programme

Modern Methods and Algorithms of Quantum Chemistry

Winterschool, 21 - 25 February 2000
Forschungszentrum Jülich, Germany

Monday, 21 February 2000

9.00-17.30	Registration
9.15- 9.45	Opening <i>Richard Wagner, Board of Directors, Forschungszentrum Jülich</i> <i>Friedel Hoßfeld, NIC, Forschungszentrum Jülich</i>
9.45-10.45	Industrial challenges for quantum chemistry <i>Ansgar Schäfer, BASF AG, Ludwigshafen</i>
10.45-11.15	Coffee break
11.15-12.45	Methods to calculate the properties of large molecules <i>Reinhart Ahlrichs, Universität Karlsruhe</i>
12.45-14.00	Lunch break
14.00-15.30	Parallel programming models, tools and performance analysis <i>Michael Gerndt, Forschungszentrum Jülich</i>
15.30-16.00	Coffee break
16.00-16.45	Basic numerical libraries for parallel systems <i>Inge Gutheil, Forschungszentrum Jülich</i>
16.45-17.30	Tools for parallel quantum chemistry software <i>Thomas Steinke, ZIB, Berlin</i>
17.30	Poster session and reception

Tuesday, 22 February 2000

9.15-10.45	Post-HF single-reference ab initio methods <i>Hans-Joachim Werner, Universität Stuttgart</i>
10.45-11.15	Coffee break
11.15-12.45	Post-HF multi-reference ab initio methods <i>Peter Knowles, University of Birmingham, United Kingdom</i>
12.45-14.00	Lunch break
14.00-15.30	Integral-direct methods, integral transformations <i>Martin Schütz, Universität Stuttgart</i>
15.30-16.00	Coffee break
16.00-17.30	R12 methods, Gaussian geminals <i>Wim Klopper, Utrecht University</i>

Wednesday, 23 February 2000

9.15-10.45	Direct solvers for symmetric eigenvalue problems <i>Bruno Lang, RWTH Aachen</i>
10.45-11.15	Coffee break
11.15-12.45	Semiempirical methods <i>Walter Thiel, MPI für Kohlenforschung, Mülheim an der Ruhr</i>
12.45-14.00	Lunch break
14.00-15.30	Hybrid quantum mechanics/molecular mechanics approaches <i>Paul Sherwood, Daresbury Laboratory, United Kingdom</i>
15.30-16.00	Coffee break
16.00-16.45	Subspace methods for sparse eigenvalue problems <i>Bernhard Steffen, Forschungszentrum Jülich</i>
16.45-17.30	Computing derivatives of computer programs <i>Christian Bischof, RWTH Aachen</i>

Thursday, 24 February 2000

9.15-10.00	Ab initio molecular dynamics: Theory <i>Dominik Marx, Ruhr-Universität Bochum</i>
10.00-10.45	Ab initio molecular dynamics: Implementation I <i>Jürg Hutter, Universität Zürich</i>
10.45-11.15	Coffee break
11.15-12.00	Ab initio molecular dynamics: Implementation II <i>Jürg Hutter, Universität Zürich</i>
12.00-12.45	Ab initio molecular dynamics: Advances <i>Dominik Marx, Ruhr-Universität Bochum</i>
12.45-14.00	Lunch break
14.00-15.30	Relativistic electronic-structure calculations for molecules <i>Markus Reiher, Universität Erlangen-Nürnberg</i>
15.30-16.00	Coffee break
16.00-17.30	Relativistic effective core potentials <i>Michael Dolg, Universität Bonn</i>

Friday, 25 February 2000

9.15-10.45	Molecular properties <i>Jürgen Gauss, Universität Mainz</i>
10.45-11.15	Coffee break
11.15-12.45	Tensor concepts in electronic structure theory: Application to self-consistent field methods and electron correlation techniques <i>Martin Head-Gordon, University of California at Berkeley, USA</i>
13.00	End of the Winterschool

Timetable

Zeit	Monday	Tuesday	Wednesday	Thursday	Friday
9:15-10:45	Opening <i>R. Wagner</i> <i>F. Hoffeld</i> Industrial challenges for quantum chemistry <i>A. Schäfer</i>	Post-HF single- reference ab initio methods <i>H.J. Werner</i>	Direct solvers for symmetric eigenvalue problems <i>B. Lang</i>	Ab initio molecular dynamics: Theory <i>D. Marx</i> Implementation I <i>J. Hutter</i>	Molecular properties <i>J. Gauss</i>
10:45-11:15	Coffee break				
11:15-12:45	Methods to calculate the properties of large molecules <i>R. Ahlrichs</i>	Post-HF multi- reference ab initio methods <i>P. Knowles</i>	Semiempirical methods <i>W. Thiel</i>	Ab initio molecular dynamics: Implementation II <i>J. Hutter</i> Advances <i>D. Marx</i>	Tensor concepts in electronic structure theory: Application to self-consistent field methods and electron correlation techniques <i>M. Head-Gordon</i>
12:45-14:15	Lunch break				
14:00-15:30	Parallel programming models, tools and per- formance analysis <i>M. Gerndt</i>	Integral-direct methods, integral transformations <i>M. Schütz</i>	Hybrid quantum mechanics/molecular mechanics approaches <i>P. Sherwood</i>	Relativistic electronic-structure calculations for molecules <i>M. Reiher</i>	
15:30-16:00	Coffee break				
16:00-17:30	Basic numerical libraries for parallel systems <i>I. Gutheil</i> Tools for parallel quantum chemistry software <i>Th. Steinke</i>	R12 methods, Gaussian geminals <i>W. Klopper</i>	Subspace methods for sparse eigenvalue problems <i>B. Steffen</i> Computing deriva- tives of computer programs <i>Ch. Bischof</i>	Relativistic effective core potentials <i>M. Dolg</i>	

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Efficient real-space approach to TDDFT for the dielectric response of periodic systems

F. Kootstra , P.L. de Boeij and J.G. Snijders

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The Netherlands*

Time-dependent density functional theory has been used to calculate the static and frequency-dependent dielectric function of non-metallic crystals. We show that a real-space description becomes feasible by using a lattice-periodic (microscopic) scalar potential in combination with a uniform (macroscopic) electric field. The induced density and microscopic potential can be obtained self-consistently for fixed macroscopic field by using linear response theory, in which Coulomb interactions and exchange-correlation effects are included. The induced polarisation (and hence the dielectric function) can then be obtained from the induced current.

We obtained the dielectric function for a wide range of materials within the adiabatic local density approximation in good agreement with experiment. The accurate results for the low-frequency range show that no adjustment of the LDA band gap seems to be necessary. Spectral features of the dielectric function appear in the calculations with the correct strength and shape, however, at more or less uniformly shifted energies.

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- ‘Efficient Real-Space Approach to Time-Dependent Density Functional Theory for the Dielectric Response of Non-Metallic Crystals’, F. Kootstra, P. L. de Boeij and J. G. Snijders.
submitted to J. Chem. Phys. 7 okt. 1999
- ‘Application of Time-Dependent Density Functional Theory to the Dielectric Function of various Non-Metallic Crystals’, F. Kootstra, P. L. de Boeij and J. G. Snijders.
submitted to Phys. Rev. B. 14 dec. 1999

Theoretical Computations of Transition Metal NMR Chemical Shifts

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Density functional theory (DFT) is now well established for the computation of NMR properties including chemical shifts of transition-metal compounds [1]. In most cases the B3LYP combination of density functionals is better suited than others to describe the shifts of the metal nuclei, $\delta(^{95}\text{Mo})$ being the only exception so far [1]. We have now extended the series of examined nuclei to include ^{49}Ti [2] and ^{99}Ru chemical shifts [3], both of which are well reproduced with B3LYP (Figure 1).

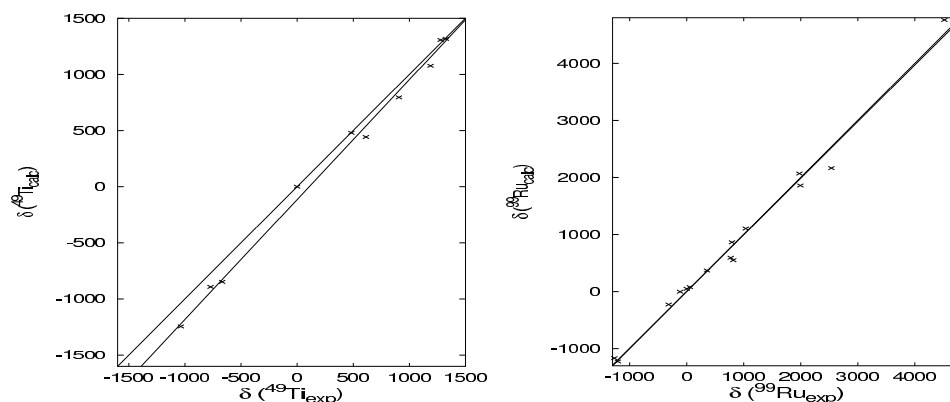


Figure 1: Computed (GIAO-B3LYP) versus experimental transition-metal chemical shifts; left: ^{49}Ti , right: ^{99}Ru . (dotted: ideal slope = 1, dashed: linear fit)

References

- [1] M. Bühl, M. Kaupp, V. G. Malkin, O. L. Malkina, *J. Comput. Chem.* **1999**, 20, 91.
- [2] F. T. Mauschick, M. Bühl, unpublished results.
- [3] M. Bühl, S. Gaemers, C. J. Elsevier, submitted for publication.

Theoretical Studies on the Higher Oxidation States of Iron

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Abstract

The stabilisation of the high oxidation states of the 3d transition metals (TM) is an important problem in inorganic chemistry. Examples are the high- T_c Cu^{III} oxides and the materials for energy storage, such as the rechargeable Li batteries based on oxides of $\text{Ni}^{\text{III}}/\text{Ni}^{\text{IV}}$, $\text{Co}^{\text{III}}/\text{Co}^{\text{IV}}$ and $\text{Mn}^{\text{III}}/\text{Mn}^{\text{IV}}$. In this contribution we report density functional (DFT) and multiconfiguration self consistent field (MCSCF) calculations on the oxo FeO_4^{2-} (Fe^{VI}) and the hypothetical oxo FeO_4^- (Fe^{VII}), FeO_4 (Fe^{VIII}) and peroxo $\text{FeO}_2(\text{O}-\text{O})^z$ [$z=-2(\text{Fe}^{\text{IV}})$, $z=-1(\text{Fe}^{\text{V}})$, $z=0(\text{Fe}^{\text{VI}})$]; $\text{Fe}(\text{O}-\text{O})_2^z$ [$z=-2(\text{Fe}^{\text{II}})$, $z=-1(\text{Fe}^{\text{III}})$, $z=0(\text{Fe}^{\text{IV}})$] and $\text{FeO}(\text{O}-\text{O})_2^z$ [$z=-2(\text{Fe}^{\text{IV}})$, $z=-1(\text{Fe}^{\text{V}})$, $z=0(\text{Fe}^{\text{VI}})$] clusters. The results show the potential of stabilising Fe^{VII} and Fe^{VIII} in tetrahedral oxo coordination. On the basis of absolute electronegativities calculated using DFT, it is predicted, that FeO_4 will be rather oxidising even stronger than Cl_2 and O_2 . Based on a comparison between total bonding energies of $\text{M}_1\text{M}_2\text{Fe}^{\text{VI}}\text{O}_4$ ($\text{M}_1, \text{M}_2=\text{Li}, \text{K}$), $\text{MFe}^{\text{VII}}\text{O}_4$ ($\text{M}=\text{Li}, \text{K}$) and $\text{Fe}^{\text{VI}}\text{O}_4$ clusters, possible synthetic routes for electrochemical preparation of FeO_4^- and FeO_4 species are discussed.

It is demonstrated that the DFT method is very powerful in calculating and predicting not only ground state but also excited state electronic structures and their properties in compounds with transition metals in their high oxidation states. Such compounds are sometimes not well characterised or at least they are synthetic targets in view of their promising properties for energy storage and energy conversion.

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Oxydation Of Methanol to Formaldehyde On V_2O_5 Investigated By Density Functional Theory.

P. Boulet^{1,2,4}, F. Gilardoni², J. Weber², H. Chermette^{1,2}, A. Baiker³ and J.-C. Volta⁴

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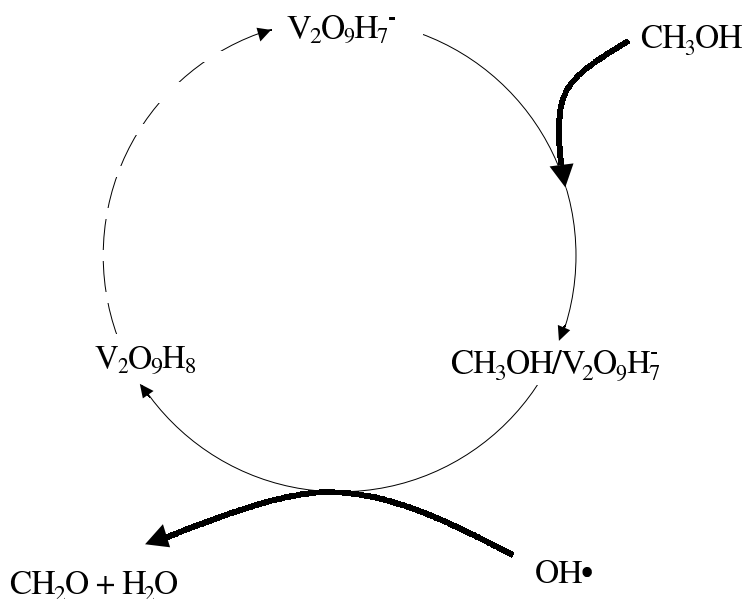
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As a precursor to materials of industrial interest formaldehyde is one of the most widely used chemicals. One way to obtain formaldehyde is to dehydrogenate methanol on vanadium oxide-based catalysts. Lots of work remain to be accomplished to understand the chemical processes of the reaction.

In this poster, we present the adsorption of methanol and propose a mechanism for the mild oxidation.



Reactivity of NO and (NO)₂ on Cu(110)

D. Voukelatos and P. J. Knowles

University of Birmingham, School of Chemistry, Edgbaston B15 2TT, Birmingham, UK

The adsorption of NO on transition metal surfaces in general shows a remarkable variety of possible bonding configurations which raises considerable interest from both chemical and catalytic point of view. The RHF and DFT methods are employed in order to calculate the energy that is required to dissociate the NO molecule from the Cu surface. According to experiment when Cu(110) is exposed to NO in the temperature range 40-85K initial adsorption leads to the presence of molecular NO on the surface. With further exposure to NO this is replaced by the dimeric (NO)₂ species. The objective of this work is to calculate the dissociation energy of Cu_xNO and Cu_x(NO)₂

Gas-phase reactions of X_3M-NCR and X_3M-CNR donor-acceptor complexes ($M=Al, Ga$; $X=H, Cl, CH_3$; $R=H, CH_3$).

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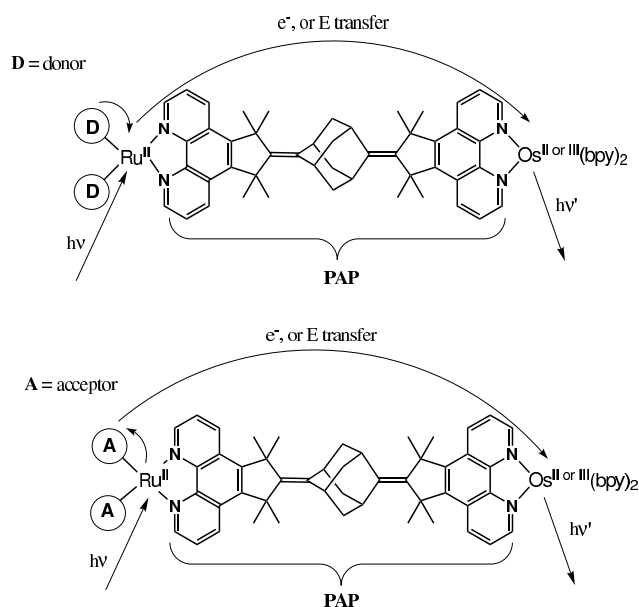
Carbon contamination is one of the major problems during the CVD of group 13 binary nitrides MN from organometallic precursors. Recently we proposed that carbon incorporation in MN is attributed to the metal-carbon bonding in the gas-phase with formation of organometallic heterocycles. To further explore processes of metal-carbon and metal-nitrogen bond formation, model complexes X_3M-NCR and X_3M-CNR ($M=Al, Ga$; $X=H, Cl, CH_3$; $R=H, CH_3$), metal cyanides X_2MCN and X_2MNC and their oligomers $[X_2MCN]_n$ ($n=2,3,4$) have been chosen for the present investigation. Geometries, relative energies, vibrational frequencies, and thermodynamic parameters of dissociation and elimination reactions are predicted at B3LYP level of theory with full-electron pVDZ basis set. All structures were fully optimized with subsequent vibrational analysis. Gaussian 94 set of programs was used throughout.

Results of this study indicate competitiveness of gallium-carbon and gallium-nitrogen bond formation. Predicted dissociation enthalpies of metal-carbon bonded complexes are about 15 kJ mol⁻¹ *higher* compared to dissociation enthalpies of metal-nitrogen bonded isomers both for Al and Ga. For X_2MCN species, Ga-C and Al-N bonding is found to be preferable compared to Ga-N and Al-C, in qualitative agreement with Pearson's HSAB concept. Relative stability of X_2MCN forms is increasing with increasing of electronegativity of terminal group X both for Al and Ga: $CH_3 < H < CN < Cl$. RX elimination reactions with dimerization of X_2MCN are extremely favorable in case of $X=H, CH_3$; in contrast, for $X=Cl$ dissociation processes are predominant.

DFT calculations for planning the synthesis of more efficient devices performing artificial photosynthesis

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Energy and electron transfer processes are very important since they are at the base of many biological phenomena, such as photosynthesis. The system showed below is an example of an inorganic device performing efficient photoinduced energy and electron transfer processes ($k_{\text{en}} = 5.2 \times 10^7 \text{ s}^{-1}$, $k_{\text{et}} = 7.2 \times 10^6 \text{ s}^{-1}$, [1]). The introduction of appropriate donor and acceptor units on the Ru(II) center can improve the lifetime of the charge/energy transfer state, resulting in a much longer and efficient storage of energy. Ab initio (DFT) calculations were made in order to predict the best donor and acceptor ligands for the synthesis of the target molecules.



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The fitting of auxiliary basis sets to electron densities.

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The effect of changing the fitting requirement for the formation of an atom-centered auxiliary basis is studied. In this case the basis (contracted gaussian functions) directly represents the electron density (i.e. the diagonal element of the one-electron density matrix) and is used within the Kohn-Sham Density Functional Theory framework to approximate two-electron (Coulomb) contributions.

The cost in terms of accuracy in using a simple density fit is investigated and compared to that the standard electric field fit advocated by Dunlap.² Exploitation of both fitting requirements has been implemented within the MOLPRO³ program.

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Density Functional Study of the 1,4-Polymerization of Butadiene with Cationic $[\text{Ni}^{\text{II}}(\text{C}_4\text{H}_7)(\text{C}_4\text{H}_6\text{PH}_3)]^+$ Complexes.

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According to the π -allyl-insertion mechanism¹ the entire catalytic cycle of 1,4-polymerization of butadiene has been theoretically studied by employing a gradient-corrected density functional method with the cationic butenylbis(ligand) complexes as the catalyst.² We have investigated competitive chain propagation cycles for generation of a cis-1,4- and trans-1,4-polymer, and also anti-syn isomerization. The calculations provide a clear insight into the stereoregulation mechanism of trans-1,4 polymerization.

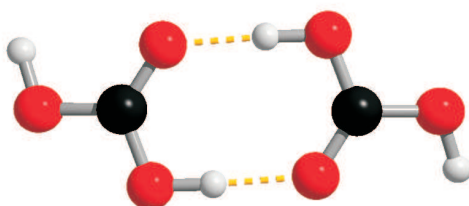
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Quantum Cluster Equilibrium Theory: Carbonic Acid in the Gas and the Solid Phase

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Despite the conventional wisdom that carbonic acid is kinetically instable, chemists recently succeeded in recognizing its stability and then in isolating and characterizing this compound. In particular, Hage et al. [1] were able to sublime and recondense carbonic acid without decomposition into carbon dioxide and water. This study could prove the stability of gas-phase carbonic acid. The vapor pressure estimates were consistent with an equilibrium mixture of monomers and dimers, comparable to that of formic acid. In this work we use the recently developed quantum cluster equilibrium (QCE) theory [2,3] at the RHF/6-31+G* and at the B3LYP/6-31+G* level of theory to calculate the equilibrium cluster population for carbonic acid in the gas and the solid phase. The validity of the resulting QCE model is tested by comparison with experimental thermodynamic and spectroscopic data.

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Simulations of the Raman Optical Activity of Peptides

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Raman optical activity (ROA) provides important information about molecular structure, stereochemistry and conformation. Thus peptides are natural target molecules for this technique. However, the interpretation of the spectra is almost entirely dependent on *ab initio* simulations, which imposes limits on molecular size and overall accuracy.

Computation of ROA is a difficult and complex process. Molecular force fields and polarizability tensors have to be calculated accurately. Currently only a slow finite difference methods can be used for evaluation of the tensors. Moreover, an origin dependence of magnetic perturbation involved in ROA has to be overcome. For peptides, another complication arises from their strong interaction with the solvent. Thus the usual vacuum-based procedures are inadequate.

Nevertheless, many of these obstacles can be overcome using suitable models and approximations. These include simplified models of the polarizabilities¹⁻² and transfer of molecular tensors.³ Currently we explore the potential of the continuum solvent models for the simulations.

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Ab initio Monte Carlo simulations of neon and argon

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Gibbs ensemble Monte Carlo simulations of neon and argon with *ab initio* pair potentials were performed. This approach is called ‘global simulation’ since quantum mechanical calculations and simulations are performed in order to obtain thermodynamic data without use of any results of experimental measurements.

During the simulations, the densities of the coexisting phases, their pair correlation functions, the vapour pressure and the enthalpy and entropy of vapourization were calculated from just above the triple point to close to the critical point. The influence of the potential choice (*ab initio* potentials, a simple and a more complex empirical potential have been compared) and of the addition of the Axilrod–Teller three-body potential on the above mentioned properties were investigated.

Phase equilibria calculated with the pair potentials studied show only a rather crude agreement with the experimental phase equilibria, but the inclusion of Axilrod–Teller three-body interaction to the potential leads to a very good agreement for all studied quantities for neon as well as for argon. For neon our simulation results for density and vapour pressure have an accuracy similar to the best presently available experimental data. It may be ventured that our simulations can supply reliable thermodynamic data of neon where no experimental data are available.

Confirmed by the good results of the calculation of phase equilibria, we studied another application of global simulations. We used simulation results to extend an equation of state for the near-critical region to higher pressure. Now the range of applicability of this equation of state is enlarged by the use of quantum mechanics and simulation.

Charge Transfer Complexes: N_4^+ , N_2CO^+ and OCCO^+

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In the dense region of planetary ionospheres, the charge transfer complexes N_4^+ [1], N_2CO^+ [2] and OCCO^+ play an important role as intermediates in the collisional energy redistribution in the diatomic fragments. Using electronic structure calculations six-dimensional potential energy functions have been generated for the electronic ground states, and one-dimensional collinear cuts for the central bond stretching coordinate in the excited states.

In the case of N_4^+ and N_2CO^+ six-dimensional variational calculations have been employed to calculate anharmonic vibrational levels for energies up to about 3000 cm^{-1} in the $^2\Sigma_u^+$ (N_4^+) or A' (N_2CO^+) electronic ground states. Apart from the two stretching modes related to the diatoms all others modes exhibit large amplitudes due to the quasi van der Waals character of the corresponding potential energy regions.

It is shown that in all three ions the first electronically excited states are $^2\Pi$ states with much smaller central bond distances than in the ground states. In the electronically excited states several conical intersections have been found.

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Intermolecular vibrational couplings in the phenol(H₂O)₁ cluster

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The intermolecular vibrations of the binary cluster phenol(H₂O)₁ are characterised by anharmonicities and strong couplings. Therefore a one-dimensional and harmonic approximation is not suitable to explain the intermolecular parts of the experimental vibrational spectra of the electronic ground state (S₀) and the first excited state (S₁). In a first step, three normal modes were chosen to perform a three-dimensionally coupled vibrational analysis of the above-mentioned system. The normal modes τ (torsional motion), β_2 (symmetric in-plane wagging motion) and ρ_1 (asymmetric out-of-plane rocking motion) were selected because the transition state of the torsion of the water molecule can be expressed with these coordinates.

An *ab initio* potential energy surface has been calculated by elongations along the τ , β_2 , and ρ_1 -coordinates. The eigenvalues of this PES were determined via the Ritz variational method. The eigenvalue spectrum as well as intensities which were obtained by the calculation of Franck-Condon factors were used to interpret experimental data. Simulated transitions were correlated with experimental bands in a frequency region of 90 to 140 cm⁻¹. The analysis of couplings depending on torsional symmetry gave valuable information about the height of the torsional barrier.

In order to simulate the intermolecular vibrations of the phenol(H₂O)₁ cluster completely, we started to perform a full six-dimensional calculation. An important basis for this is an *ab initio* potential energy surface at a high level of theory. The hamiltonian to solve the eigenvalue problem will include monomer parts and coupling terms to describe the couplings between the motions of the two monomers as well as interactions with the overall rotation [1].

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REACTIVITY OF *ANTI*-O,O'-DIBENZENE RADICAL CATION IN ARGON MATRIX

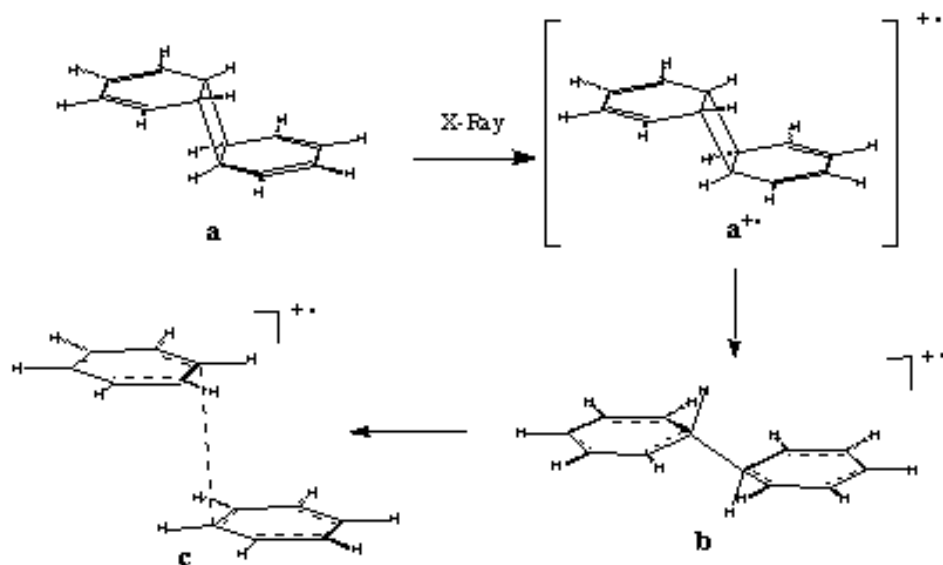
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Neutral dibenzene **a** on standing at room temperature slowly cleaves into two molecules of benzene. In the case of the radical cation, other modes of rearrangement are considerable, like a cleavage of a single bond. However, after X irradiation of a sample kept at low temperature in an Ar matrix, a band at 920 nm is found, which is due to the dimer cation $(C_6H_6)_2^+$, **c**.

Calculations on possible intermediates and products of dissociation of $\mathbf{a}^{\cdot+}$ support the idea that the parent radical cation is instable under the condition of its generation. The reaction path is characterized by the initial scission of one bond between the two rings of **a** giving, with a barrier of few kcal/mol, the species **b** which relaxes, after a state crossing, to the dimer cation **c**. B3LYP/6-31G* method was used to map the energy profile of the process. Moreover, state diagrams were derived to depict how the relevant electronic states correlate along the dissociation path. For this case, all stationary points were recalculated at CASSCF(10,9) with an A.N.O. basis set, and dynamic correlation was introduced by the CASPT2 method.



BROADENING AND POLARISATION OF D1 AND D2 LINES OF SODIUM INDUCED BY COLLISIONS WITH ATOMIC HYDROGEN

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The broadening of lines by collision with atomic Hydrogen is directly related to electrostatic interaction potentials correlated to atomic states of the line. The elements chosen are abundant elements used for the spectroscopic diagnostics in stellar astrophysics : alkaline-earth elements and alkalis. The results presented here are relevant to D1 and D2 lines of Sodium perturbed by Hydrogen under the solar photosphere physical conditions (temperature : $T = 5000\text{K}$). The following steps are involved :

- calculation of interatomic potentials using modern methods in quantum chemistry. Indeed the use of approach potentials (Van Der Waals, for example) only gives the right order of magnitude of the broadening, but the sensitivity of present detectors now requires an improvement on the theoretical results that can be provided by *ab initio* potentials and more refined line broadening calculation.
- collision calculation which gives all cross sections and collision amplitudes.
- calculation of depolarizing cross sections and line broadening : a theoretical treatment of the multipole relaxation and transfer rates due to isotropic collisions is presented. Explicit expressions are obtained for the rate constants of the Na ground state hyperfine levels perturbed by collisions with H atom.
- links and comparison with astrophysical observations

Laserinduced Desorption of CO from Chromiumoxide

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In recent experiments the rotational alignment of the laserinduced non-thermal desorption of CO adsorbed on an epitaxially grown film of Cr_2O_3 (0001) has been studied[1]. At low rotational quantum numbers J the molecules desorb like a helicopter (J-vector perpendicular to the surface) while at high J -values a cartwheel motion is preferred (J-vector parallel to the surface).

These stereodynamical effects and the experimental state resolved velocity distributions of the desorbing species are simulated using a time dependent wave packet method in four dimensions. As a prerequisite for these investigations substantial effort had been necessary in the field of development and implementation of efficient algorithms for the solution of the time-dependent Schroedinger equation in many dimensions. Up to four dimensional wave packet calculations including diabatic coupling elements and arbitrary laser pulses can be performed using the computer equipment available in our department. A high dimensional version of our code for the use on massively parallel platforms (Cray T3E) has been developed.

As a basis for this quantum mechanical treatment of nuclear motion of the adsorbed molecule a fourdimensional ab initio potential energy surface for the electronic ground state of this adsorbate-substrate system has been calculated in an embedded cluster approach[2]. Different slices through electronically excited states are calculated in a configuration interaction scheme and the influence of several coordinates on the final state distributions is examined[3]. To improve the quality of these quantumdynamical simulations, a fourdimensional ab initio potential energy surface for an electronically excited state is modelled at the moment. The basis for this PES is an internal $5\sigma - 2\pi$ excitation within the adsorbed CO molecule.

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Vibrational spectra from data of subsystems

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Although NMR spectroscopy and X-ray analysis are the most widely used analytical tools in a synthetically oriented lab, vibrational spectroscopy is still of importance. An advantage of IR spectroscopy, especially when compared to NMR spectroscopy, is that it has a much higher sensitivity and that it can be performed faster. A major disadvantage, however, is that there is no direct way from the spectrum to structural features of the system studied. Therefore the well established method of structure elucidation by means of vibrational spectroscopic data is the comparison of calculated and experimental spectra. Using this approach in combination with NMR spectroscopic data one can often do calculations on smaller systems, e.g. systems which have a substituent as t-butyl replaced by methyl (or even hydrogen). This, of course, does not work in the case of vibrational spectroscopy. One always has to perform a calculation on the 'full' system including all substituents and groups. Despite the successes in computer technology as well as in the area of code development which lead to higher and higher performance of the programs used there are always molecules which are too large to perform calculations of a sufficient accuracy on.

Within the approach we present here the hessian of the target molecule is built up from the Hessians of smaller systems, e.g. parent compound + models of substituents, (overlapping) parts of the target molecule. The built up process is done using the so-called 'primitive internals', i.e. a full set of valence coordinates, stretches, bends and torsions [1]. Internal coordinates, especially redundant internal coordinates, have recently been used successfully not only in geometry optimizations but also to scale the calculated force constants [1].

The built up process will work well only if the force constants are transferable from the source molecules to the target and if the couplings between the parts of the target system represented by different source molecules are negligible.

We discuss some illustrative examples, e.g. substituted diphosphenes, heterocubanes, porphines and aromatic compounds. They fulfill the requirements mentioned to a different degree.

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Adsorption of Polyacrylic Acid on Aluminium Oxide: DRIFT Spectroscopy and Ab Initio Calculations

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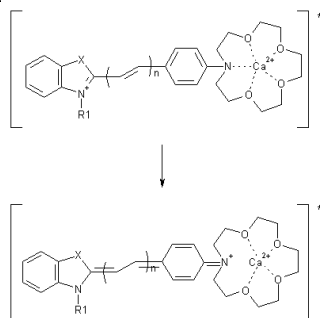
Abstract

Diffuse reflectance Fourier transform infrared (DRIFT) spectroscopy was used to study the adsorption process of the water-soluble polyacrylic acid (PAA) polymer on hydrous δ - Al_2O_3 . Vibrational assignment of PAA, sodium polyacrylate (Na-PA) and the PA-oxide surface complex was achieved by comparison of observed band position and intensity in the DRIFT spectra with wavenumbers and intensities from ab initio quantum mechanical calculations. The presented data of polyacrylic acid suggest that IR data calculated ab initio on relatively short oligomers may provide valuable information regarding the interpretation of polyelectrolyte infrared spectra.

Batch experiments were performed to adsorb PAA onto the δ - Al_2O_3 surface. The results obtained from DRIFT studies were compared with adsorption isotherm experiments in order to relate the level of PAA coverage to the nature of the surface complex. Ab initio molecular orbital calculations on PAA/ Al_2O_3 clusters were used to model possible surface complexes. Strong correlation were found between theoretical and observed DRIFT frequencies of the antisymmetric R-COO⁻ vibration. A number of possible configurations of the polyacrylic acid/aluminate surface complex were tested via ab initio calculations. These possible configurations included different di-aluminium octahedral Al^{3+} surface models. Results obtained from adsorption isotherm experiments, DRIFT spectra and ab initio calculations indicate that the carboxylate oxygens bridge an Al^{3+} -octahedral dimer [$\text{Al}_2(\text{OH})_2 \bullet 4(\text{H}_2\text{O})2(\text{OH})$] in a ligand-exchange inner-sphere complex.

A model study of photoinduced recoordination in cationic complexes of photochromic azacrown ethers

Crown ether styryl dyes are known to undergo photoinduced trans-cis isomerization or [2+2]-cycloaddition [1]. Complex formation with metal cations affects the efficiency of these reactions. On the other hand, complex formation of these dyes is photocontrolled, which makes possible the use of these systems as sensors or molecular machines. An interesting case of photoinduced changes was observed in styryl and butadienyl dyes containing N-phenylazacrown ether moiety (see [figure](#)). UV absorption spectra of the dyes indicate that photoinduced recoordination occurs in their complexes with metal cations; that is, M–N bond breaks, and the cation moves from the position in the center of the cavity towards the oxygen atoms [2, 3]. Theoretical consideration shows that this recoordination is necessarily followed by a conformational change. Moreover, the recoordination cannot be observed if the conformation of the crown ether moiety is constrained. It is believed (and supported by ¹H NMR studies) that recoordination and conformational change are caused by electron density redistribution upon photoexcitation.



One can see that the participation of the quinoid resonance form should induce the charge transfer from the heterocyclic N atom to the N in the crown ether thus reducing the binding capacity of the latter. To simulate these changes, the following molecules were taken as models: (1) N-phenylaza-15-crown-5 and (2) its quinoid analog.

Our experience of application of different methods to crown ethers [4] shows that a reliable conformational study is possible using rough *ab initio* methods (like RHF/3-21G), whereas the detailed study of complex formation including formation energies is possible only when the electron correlation is included (MP2/6-31G*, DFT). However, neither semiempirical nor molecular mechanical simulations can give us the insight into the problem. Therefore, we chose the large-core SBK pseudopotential basis set for our RHF calculation.

It was found that (1)Ca²⁺ complex assumes the "axial" conformation with the phenyl ring in the axial position to the average plane of the crown ether and has five binding sites, whereas (2)Ca²⁺ complex assumes the "equatorial" conformation with the phenyl ring in the equatorial position to the crown ether plane and has four binding sites. The axial conformation of (2)Ca²⁺ also exists but lies ~4.4 kcal/mol higher. The fact that (2)Ca²⁺ has only four binding sites explains its lower formation energy as compared to (1)Ca²⁺. This is consistent with the stability constants found for the cation–dye complexes and compared to those for N-phenylaza-15-crown-5.

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Parallel Implementation of the Self-Consistent-Charge Density-Functional-Based Tight-Binding

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The density-functional-based tight-binding method with charge-selfconsistency (SCC-DFTB) has been applied to a variety of problems in the fields of solids, surfaces, inorganic clusters and even biological molecules. This fast and efficient method has proved to be very accurate, results are usually in very good agreement with fully self-consistent DFT results.

The method has been implemented for parallel computers based on MPI and Scalapack and was tested on various hardware including the T3E and PC-based distributed-memory computers. We present details about the performance and scaling behaviour and demonstrate applications of the parallel code.

Electronic Structure Computation on a NUMA Parallel Supercomputer

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We investigate strategies for the optimal exploitation of a parallel computer consisting of clusters of shared-memory-parallel (SMP) nodes, using molecular electronic structure theory (triple-excitation component of many-body perturbation theory) as the example. Although inter-node communication must be handled using a message-passing paradigm, within the node more direct use of shared memory is possible. This leads naturally to the coding of hierarchical parallel algorithms, in which coarse-grained division of work between nodes (handled in our code by the the Global Arrays (GA) toolkit) encloses finer-grained parallel structures that can be conveniently programmed using OpenMP. An alternative strategy is to simply use GA in a single-level parallel implementation, and it is not clear from the outset whether this simpler approach is better or worse than the nested method. Comparative results on an 8-node 2-way-SMP IBM SP computer illustrate the relative performance of the two algorithms.

PERFORMANCE OF PARALLEL SYMMETRIC EIGENSOLVERS IN QUANTUM CHEMISTRY CODES ON CRAY T3E

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Nearly one-third of the projects on the Cray supercomputer complex in Jülich pertain to the area of computational chemistry. For projects in quantum chemistry ZAM offers several extensive software packages running on CRAY T3E [1]. The solution of the symmetric eigenvalue problem is a compute-intensive task in many quantum-chemical calculations. We studied the performance of symmetric eigensolvers from different parallel libraries on CRAY T3E: GA_DIAG_STD from Global Arrays used in NWChem [2] (calling PDSPEV from PeIGS), PSSYEVX from ScaLAPACK contained in the Cray scientific library and used in DGauss [3], and PSSYEV from the public domain version 1.6 of ScaLAPACK. All eigensolvers use the following three-step-algorithm:

1. reduction of the full symmetric matrix to tridiagonal form;
2. solution of the tridiagonal eigenproblem;
3. back transformation of the eigenvectors.

PSSYEVX and PDSPEV use bisection and inverse iteration for the solution of the symmetric tridiagonal eigenproblem, in PSSYEV a modified QR-algorithm is applied. PDSPEV uses a parallel version for the reorthogonalization of eigenvectors whereas PSSYEVX does reorthogonalization of all eigenvectors belonging to one cluster of eigenvalues on a single node. This means that for large clusters of eigenvalues reorthogonalization with PSSYEVX is not possible because of memory exhaustion.

If there are no large clusters of eigenvalues or if reorthogonalization is not needed then PSSYEVX is significantly faster than PDSPEV as it is written in a blocked version using BLAS 3 and BLAS 2 operations whereas PDSPEV is based on BLAS 1 routines. On machines with small level 1 caches only the use of BLAS 3 routines can deliver good performance. If eigenvectors for large clusters of eigenvalues are needed orthogonal to a high precision then PSSYEV from ScaLAPACK is the best performing routine. The eigenvalues of the tridiagonal matrix are computed simultaneously on all processors and the eigenvectors are computed in parallel.

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MBPT AND DFT STUDIES OF HYDROGEN CYANIDE BORANE(1) OLIGOMERS, POLYMERS AND THEIR DEHYDROGENATED ANALOGS

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The idea of hydrogen cyanide borane(1) polymer is closely related to our previous calculations^[1] of the formation of the dimer (HCNBH)₂. The open-chain planar E-isomer of (HCNBH)₂ exhibits remarkable thermodynamic stability and can be considered as the starting point for the modeling of the polymer (Fig.1). We also propose the model with two-coordinate boron (Fig.2).

Geometry optimizations and fragmentation energies of the series of oligomers based on these two structural models are performed with the aim to find the suitable reference cell of polymers for a finite-periodic-cluster (FPC) calculations of band gaps.^[2] Geometry of the oligomers is examined at different computational levels: MBPT(2) (second-order Many-Body Perturbation Theory), SDQ-MBPT(4) (fourth-order Many-Body Perturbation Theory limited to singly-, doubly- and quadruply excited configurations) and DFT-B3LYP (Density Functional Theory with Becke's three parameter hybrid functional using the LYP correlation functional). Both models seem to be suitable for the polymer chain construction, because of their periodic structure emerging from successive HCNBH or HCNB addition. The stability of the oligomers (up to pentamers) with respect to the decomposition to various fragments is fairly high ranging from 111 to 441 kJ/mol for the HCNBH series and from 345 to 606 kJ/mol for the HCNB series. These fragmentation energies are related to the rupture of the weakest bonds (based on the bond order analysis).

One can consider our two polymer models as the derivatives of polyacetylene (which is widely studied for its interesting properties) and anticipate the impact of electron-donor and electron-acceptor parts in the potential polymer chain to its band structure, and hence to its possible electrical conductivity.^[3,4] The band gap for our HCNB model polymer is 2.6 eV, which is smaller than the band gap for polyacetylene calculated by the use of the same level of theory: 3.8 eV.

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Photodissociation study of Cyclopentadienyl Manganese Tricarbonyl $[\text{CpMn}(\text{CO})_3]$ based on ab initio potentials

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The different dissociation channels of a bi-ligand transition metal compound, $\text{MnCp}(\text{CO})_3$, are investigated in the gas phase. Recent experimental studies¹ suggest that carbonyl elimination takes place in a femtosecond time scale. On this poster we present the analysis of the excitation spectra of $\text{MnCp}(\text{CO})_3$ and the potential energy curves that connect the electronic ground state and the excited states of the reactant to those of the primary products, obtained by quantum chemical methods. In a second step, time-dependent quantum wave packets will be propagated in order to control by mode selectivity the competitive bond breaking pathways.

Quantum ab initio calculations have been carried out under C_S symmetry constraint assuming a staggered conformation in the rotation of the $\text{Mn}(\text{CO})_3$ group with respect to the Cp ring. Complete active space self consistent field (CASSCF) optimizations have been performed for the electronic ground state and a few low-lying excited states. Multiconfigurational second order perturbation (CASPT2 and MS-CASPT2) Frank-Condon energies and CASSCF transition dipole moments for the lowest singlet states are compared with those obtained by time-dependent density functional theory (TD-DFT). CASSCF and MS-CASPT2 potential energy curves have been calculated for one and two synchronous CO dissociation. The Mn-CO bond cleavage seems to occur via a directly repulsive metal centered excited state corresponding to a $3d \rightarrow 3d$ excitation.

¹ *P. Rosendo-Francisco, S. Vajda and L. Wöste, private communications.*

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Electronic structure of MX and MX₂ systems

(M = Cu, Ag, Au, X = F, Cl, Br)

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Potential energy functions of systems including a metal atom, and one or two halogen atoms (MX or MX₂), have been studied by ab-initio calculations.

In the present study, relativistic pseudo-potentials optimized in the group of H. Stoll (University of Stuttgart) were used. All molecular systems of interest were studied with similar linear space of configurations, considering only the highest two occupied electron shells. MRCI potential functions of the low-lying electronic singlet and triplet states, the dipole moment functions and the spectroscopic constants were calculated for the nine MX molecules. The results are compared with existing experimental data and previous theoretical calculations. The energy gap between the ground state and the excited states increases as the ionic character of the metal-halogen bond decreases, going from Cu to Au, whatever the halogen is.

Collinear cuts of the potential energy functions for MX₂ systems were obtained at the CCSD(T) or at the MRCI level of theory. Calculations of the three dimension potential energy functions and of the geometry dependence of the spin-orbit coupling for the lowest doublet states are in progress.

Quantitative prediction of gas-phase ^{13}C NMR chemical shifts

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The accurate prediction of NMR chemical shifts is still a great challenge. While typical errors in SCF ^{13}C chemical shift calculations are about 5-10 ppm, application of correlated methods reduces the errors significantly. Nevertheless it has so far not been possible to predict chemical shifts with an accuracy of about 1 ppm or better and thus to reach quantitative accuracy compared to experimental gas phase NMR data.

In this study we demonstrate that this accuracy can be achieved if :

- chemical shifts are calculated at CCSD(T) level using large basis sets, e.g. of pentuple zeta quality augmented by higher angular momentum functions,
- employed molecular geometries are taken from CCSD(T) optimizations using sufficiently large basis sets such as cc-pVTZ or cc-pVQZ,
- vibrational corrections to chemical shifts are included.

Calculations of ^{13}C chemical shifts for a set of 15 small organic compounds containing different types of bonding environments are presented. A detailed study of the effects of correlation level, basis set convergence and the need of vibrational corrections is carried out in order to reach a maximum deviation of less than 1 ppm.

The results are compared to experimental gas phase ^{13}C NMR data.

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Ab initio treatment of electron correlations in polymers: lithium hydride chain and beryllium hydride polymer

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Correlated *ab initio* electronic structure calculations are reported for the polymers lithium hydride chain $[LiH]_{\infty}$ and beryllium hydride $[Be_2H_4]_{\infty}$. First, employing a Wannier-function-based approach, the systems are studied at the Hartree-Fock level, by considering chains, simulating the infinite polymers. Subsequently, for the model system $[LiH]_{\infty}$, the correlation effects are computed by considering virtual excitations from the occupied Hartree-Fock Wannier functions of the infinite chain into the complementary space of localized unoccupied orbitals, employing a full-configuration-interaction scheme. For $[Be_2H_4]_{\infty}$, however, the electron correlation contributions to its ground state energy are calculated by considering finite clusters of increasing size modelling the system. Methods such as Møller-Plesset second-order perturbation theory and coupled-cluster singles, doubles and triples level of theory were employed. Equilibrium geometry, cohesive energy and polymerization energy are presented for both polymers, and the rapid convergence of electron correlation effects, when based upon a localized orbital scheme, is demonstrated.

Spin-Restricted MBPT and CC Theory

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Coupled Cluster calculations for open-shell systems with an unrestricted Hartree-Fock reference (UHF) are usually suffering from spin contamination and are too expensive (by a factor of 3 to 4) in comparison to the corresponding restricted Hartree-Fock (RHF) calculations. Szalay and Gauss (*J. Chem. Phys.* **107** [1997] 9028) proposed a solution to both problems via the so-called spin restricted (SR) theory, i.e. an approach that introduces additional constraints via projected spin equations. These constraints lead to a reduction of the number of independent amplitudes and thus allow a reduction of the computational effort (within an efficient implementation). Additionally, the CC spin expectation value is equal to the exact spin expectation value even though the wavefunction is not rigorously spin adapted.

In this work we present the extension of the SR-CC-approach — which has initially been derived and implemented only for doublet cases — to triplet- and quartet-cases. Furthermore, analytical gradients for the SR-CC approach are presented along with a „spin-restricted“ variant for many-body perturbation theory (MBPT). Exemplary calculations demonstrate the quality of the results that can be achieved with SR-CC and SR-MBPT.

Basis-set convergence in correlated calculations of molecular properties

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Abstract

An investigation of the basis-set convergence of the correlation contribution to the interaction energy of hydrogen-bonded complexes (ΔE_{corr}), to the molecular electric dipole moment (μ_{corr}), and to the relativistic two-electron Darwin term (D_{corr}^{2e}) is presented. For the correlation-consistent basis sets, the convergence of ΔE_{corr} and μ_{corr} follows an X^{-3} -form in the cardinal number X similar to the one for the correlation energy once other significant basis-set errors than those originating from the incomplete description of the electronic Coulomb cusp have been addressed—i.e., diffuse basis functions have been included in the basis set and, in the case of ΔE_{corr} , the counterpoise correction has been applied. The convergence of D_{corr}^{2e} follows an X^{-1} -form, and the observed different rates of convergence are rationalized within a general theory framework for basis-set convergence.

CASSCF AB INITIO STUDIES OF ORGANIC PEROXIDE AND HYDROPEROXIDE FORMATION BY SINGLET OXYGEN ADDITION TO UNSATURATED AND AROMATIC COMPOUNDS

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Singlet-oxygen addition to unsaturated and aromatic compounds plays an important role in the peroxidation processes that occur in living organisms. Many theoretical studies were carried out of the 1,2-addition, but only one MINDO/3-CI and one *ab initio* UMP2 study of oxygen addition to butadiene and one semiempirical and DFT study of oxygen addition to benzene were reported, but no study was carried out at the MCSCF level. Therefore we devoted our present study to the cycloaddition reactions of the singlet ($^1\Delta_g$) oxygen to *cis*-1,3-butadiene and benzene, respectively, with the formation of 1,2-dioxo-cyclohexene-4 (models of oxygen 1,4-cycloaddition to conjugated compounds) by means of the CASSCF/MCDQPT2 *ab initio* method with the 6-31G* basis set. In the case of butadiene the reaction is exoenergetic and the product has a C_2 symmetry, with the peroxide moiety in the *gauche* configuration. In the case of benzene the reaction is endoenergetic and the tricyclic product formed has a C_{2v} symmetry with the peroxide moiety in the *syn* configuration. Three possible reaction routes were studied: i) concerted cycloaddition, ii) two-stage cycloaddition with the formation of a five-membered ring peroxirane intermediate, and iii) two-stage cycloaddition with the formation of a linear intermediate. In the case of butadiene routes i) and ii) were excluded, because only second-order saddle points were found on the corresponding reaction pathways. The linear intermediate (I1) found on route iii) has a biradicaloid character and its relative energy is 4.09 kcal/mol, taking into account the basis set superposition error (BSSE). The dominant activation barrier corresponds to the transition state TS1 leading to I1 and amounts to 13.5 kcal/mol. The rearrangement of I1 to the product (P) involves only a minor activation barrier of 3.5 kcal/mol (relative to I1). In the case of benzene the concerted binding mode is favored, the activation barrier being 25.25 kcal/mol. This difference in binding mechanism can be explained in terms of the configuration of peroxide moiety in the adduct.

Supported by the Polish State Committee for Scientific Research. Calculations were carried out with the use of the resources and software at the Interdisciplinary Center for Molecular Modeling (ICM), Warsaw, Poland, the Informatics Center of the Metropolitan Academic Network (IC MAN) at the Technical University of Gdańsk, and the IBM RS/6000 workstation at the Institute of Physics of Nicholas Copernicus University.

The Effect of Solvation on the Excited States of Water and Methanol.

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The study of the electronic structures/spectra of solvated systems is more difficult than their gas counterparts due to the complex nature of solute-solvent interactions. In this work the effects of solvation on the excited states of water and methanol are investigated. The excitation energies of the five singlet excited states of water complexed with a water molecule, and of the first three singlet excited states of methanol also complexed with one molecule of water are computed using ab initio methods: MCSCF, CASPT2, MRCI and the Coupled Cluster- Linear Response Theory, also known as Equation of Motion, EOM-CCSD. The possible solvatochromic shifts are investigated.

Ab initio Calculations of the Chiroptical Properties of Z-Configured Polymethine Dyes

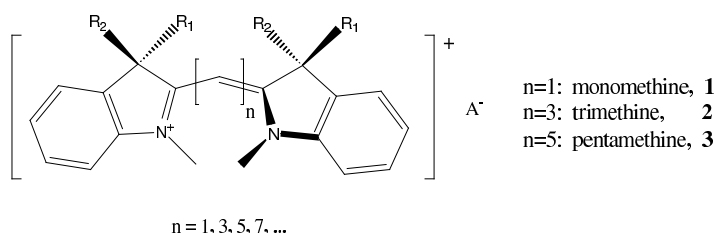
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Ab initio calculations of a series of inherently chiral, all-Z-configured polymethine dyes



are presented. The experimentally known chiroptical properties of the monomethine **1** and trimethine **2** make these compounds and their homologue **3** ideally suited to test the applicability of quantum mechanical calculations.

In compound **1** the chromophore is forced into a twisted all-Z-conformation by steric interaction of the end groups, while in **2** the presence of a t-butyl group in the *meso*-position enforces this conformation, which is manifest in the UV/Vis spectra not only in the reduced intensity of the longest wavelength absorption (methine band), but also in the occurrence of a „cis-peak“ at shorter wavelengths^[1].

Using the *MOLCAS* program-package excited states were calculated with the *CASSCF* and *CASPT2* methods. Electric and magnetic dipole transition moments were calculated, yielding UV/Vis and CD-spectra in good agreement with experimental results. The negative sign of the CD-band observed for P-helical monomethine **1** which appears to violate established helicity rules can be understood with the aid of a component analysis^[2,3] and was confirmed by the quantitative calculations. Additional calculations on the as yet not synthesized pentamethine **3** allow to predict the theoretical spectra of this compound.

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AB INITIO STUDY OF REACTION MECHANISM OF OZONE WITH ETHENE AND ITS MONOHALOGENATED DERIVATIVES

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The reactions with ozone, beside the reactions with hydroxyl and nitrate radicals, represent the most important tropospheric sink for biogenic and anthropogenic alkenes. For that reason, in the past 40 years a number of studies have dealt with their kinetic and mechanistic aspects. Although the overall kinetics of these reactions is largely known nowadays, there is still a considerable uncertainty regarding their detailed mechanisms and product yields. In this work ab initio CASSCF and CASPT2 methods were employed in studying the reaction mechanisms of ozone with ethene, fluoro- and chloroethene up to the formation of the primary addition product (ozonide). Structural and electronic properties of the reactants, transition states and addition products were determined and discussed. Also given are the analyses of kinetic parameters in terms of the simple transition state theory (TST). Finally, in case of the ozone addition to ethene, reaction path study (IRC) was carried out and led to the determination of an approximate structure of the pre-reaction van der Waals complex. Whenever possible, a comparison is made between the theoretical and experimental values and these are generally in a good agreement.

Towards reliable conformational energies: hexane conformers

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The fact that both many small molecules and in particular macromolecules can adopt a variety of different conformations is of eminent relevance with respect to their properties. The precise geometry and the relative energies of different conformations of small molecules have been the issue of many studies in the past. Small molecules can usually be studied in the gas-phase, and their structure can be experimentally resolved in great detail [1]. Quite some problems still remain to be solved, however, in particular when no direct experimental access is available. It is in those cases that first-principles or ab-initio type calculations can be of great value. In addition, ab initio based information has an important additional value in the development of empirical potentials, e.g. force fields, for large molecules like (bio)polymers, which are generally based on potential energy surfaces of similar, monomer-like, fragments.

The alkanes belong to a class of very simple molecules, while a polymeric form, polyethylene, is the simplest polymer. The all-trans conformation is the energetically most stable form. However, in the liquid state and in the amorphous polymer the fraction of gauche bonds increases (of the order of 40% at ambient temperature). Experimentally, a single isolated gauche bond is about 0.5 kcal/mol [1,2] less stable than the trans bond. Whereas the relative energy of a chain with gauche bonds increases with the fraction of gauche bonds, this increase is not purely additive in the number of gauche bonds, particularly not when the gauche bonds are neighbours or next-nearest neighbours in the alkane or polyethylene chain.

It appears generally accepted that the energy of a conformer becomes less favourable with increasing gauche content. However, in a theoretical study Frey et al. [3] reported the surprising result that the ggg conformer in hexane is more stable than the gtg conformer. Although somewhat counterintuitive, this result has been extracted from the highest level of ab initio calculations reported on hexane until 1999.

In order to investigate the somewhat unexpected result reported by Frey et al. in more detail, we have applied Hartree-Fock and post-HF methods to evaluate the relative stability of these conformers. We find that at levels higher than MP2 the gtg conformer is found more stable than the ggg conformer, in agreement with the conventional idea that each additional gauche bond causes a further decrease in stability of the conformer. DFT methods were also applied, but although DFT methods including gradient corrections show correct qualitative behaviour, quantitatively the relative energies are far off compared to the post-HF results.

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Potential energy functions and rovibrational spectra of the diaza- dicarbon (CCNN) and cyanogen (NCCN)

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The six dimensional PEFs of the ground state of CCNN and NCCN has been generated by the RCCSD(T) approach. The quartic force field in dimensionless normal coordinates has been evaluated. This force field has been used to calculate a set of spectroscopic constants. For NCCN, the quartic force field has been optimised using the experimental results and the full rovibrational spectrum is given with an accuracy better than 1 cm^{-1} . In the case of CCNN, the lowest singulet states are investigated. The ground state ($X^1\Sigma^+$) is found to be stable against dissociation into C_2 ($X^1\Sigma_g^+$) and N_2 ($X^1\Sigma_g^+$) and it presents a potential energy barrier due to an ovoided crossing with the excited $d^1\Sigma^+$ state. The other singulet states are found to be repulsive with respect to the dissociation into C_2 and N_2 .

***Ab initio* investigation of the ground state of C₃H⁻: Potential energy function and rovibrational spectrum**

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Neutral unsaturated carbon chains and their ions have been the subject of much recent interest owing to their potential role in the chemistry of the interstellar medium. The detection of spectra for such species and their interpretation is greatly aided by simultaneous theoretical studies.

This poster presents a six–dimensional *ab initio* potential energy surface (PES) for the ground singlet state of C₃H⁻ generated using the CCSD(T) method and the aug–cc–pVQZ basis set. In agreement with previous studies, the global potential minimum corresponds to a cyclic isomer (C_{2v}, R_{CC}=1.380 Å, R_{CC}=1.380 Å, R_{CH}=1.083 Å, C[∧]CH =46.9°) and a local minimum is also located, about 2500 cm⁻¹ higher in energy, corresponding to a planar trans bent isomer (C_s, R_{CC}=1.363 Å, R_{CC}=1.289 Å, R_{CH}=1.110 Å, C[∧]CC =109.2°, C[∧]CH =171.7°). The PES, represented by a fitted analytical form in the region of the two minima, is used in variational calculations to determine anharmonic rovibrational term values for both isomers and their deuterated analogues. Rotational, centrifugal distortion and vibration–rotation constants are also evaluated.

Molecular electrostatic field as useful descriptor of molecular lipophilicity

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Lipophilicity is of considerable interest for the prediction of transport, adsorption and distribution properties of molecules and as such, represent an important factor in drug design [1]. According to very complex nature of lipophilicity, sophisticated and time consuming simulations are necessary for quantitative treatment. In this study the simple method for qualitative description of molecular lipophilicity based on statistical analysis of molecular electrostatic potential (MEP) and molecular electrostatic field (MEF) are proposed.

The triangulated solvent excluded surface (vertices + faces) were generated with MSMS [2] program. The additional six points for each vertices at the molecular surface were generated due to numerical calculation of molecular electrostatic field. MEP and MEF at those points were calculated using modified MOPAC 97 [3] and AM1 and PM3 model were applied. The statistical analysis and VRML graphical representation of MEP and MEF at the molecular surfaces were made by homemade programs.

The descriptors obtained with the statistical analysis of MEP and MEF show good agreement with the experimental logP values for model compounds: acids, alcohols, amines and hydrocarbons. The VRML graphical representation of MEF is very useful for localisation of molecular lipophilicity.

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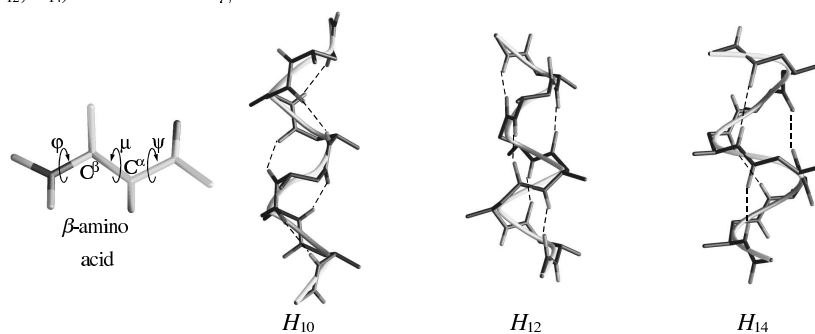
Substituent Effects on the Folding of β -Peptides

Robert Günther,^a Krzysztof Kuczer,^b Hans-Jörg Hofmann^a

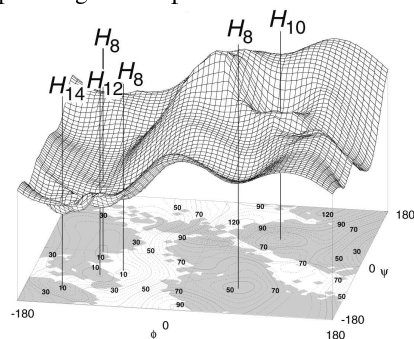
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Oligomers of β -amino acids, called β -peptides, have attracted much attention in the last few years as an interesting extension of the growing class of peptidomimetics. Compared with α -peptides, these oligomers of β -amino acids have an extra CH_2 -group in the backbone of each residue. Surprisingly, the incorporation of the additional C^β -atoms considerably stabilises characteristic secondary structures. Among the numerous types of these structures, for instance β -sheets and turns, various types of β -peptide helices differing by the size of the hydrogen-bonded cycles and handedness (e.g. H_{10} , H_{12} , H_{14}) are most striking.



In comparison with common α -amino acids, β -amino acids offer a wider variety of substitution patterns, which are expected to have significant influence on the stability of the different β -peptide helices. We present a quantum chemical study on the substituent influence on the folding tendencies in β -peptides employing *ab initio* MO theory. The study is completed by calculating free energy gradient maps of various β -peptide hexamers on the basis of molecular dynamics using the CHARMM force field. These free energy gradient maps inform on the folding possibilities of the β -peptide oligomers dependent on the substitution type as illustrated for Ac- $[\beta^3\text{-HAla}]_6\text{-NHMe}$:



Reduced free energy surface of the blocked hexamer Ac- $[\beta^3\text{-HAla}]_6\text{-NHMe}$ in vacuum

DFT-MRCI Hybrid Theory

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Many electronic structure problems are localised in the sense that the important electronic effects that influence a prediction can be viewed as occurring in a small region of space, or a subset of molecular orbitals. We split the overall orbital space of a system into two partitions, A and B , where A contains the chemically active orbitals. The spectator partition, B , is represented using an inexpensive low-level theory (eg. density functional theory (DFT)). At a cost comparable to that of using a high-level *ab initio* method, eg. multireference configuration interaction (MRCI), on A alone, we minimise an energy expression for the total system of the form,

$$E_{A\oplus B} = E_{A\oplus B}^{DFT} - E_A^{DFT} + E_A^{MRCI}.$$

The coupling between A and B arises properly through the variational minimization of the overall energy functional.

Toward Quantitative Prediction of Stereospecificity of Metallocene-Based Catalysts for α -Olefin Polymerization

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The *qualitative* relationship between the local structure of the *ansa*-metallocene catalysts and the resulting polypropene can readily be addressed through e.g. simple symmetry-rules¹ and molecular mechanics calculations², whereas the question of to what extent the tacticity of the polymer actually can be *quantitatively* predicted through independent means has not received much attention.

We are currently investigating to what extent combined approaches may contribute to the accuracy of such predictions,^{3,4} and we have started out by taking the simplest possible approach: energies of four different (diastereomeric) transition states of propene insertion into the zirconium-polymer bond are obtained using molecular mechanics (MM) geometry optimizations utilizing a frozen central geometry (termed aggregate) taken from a density functional theory (DFT) calculation.

To enable a quantitative comparison with experiment, the energy of the diastereomeric models of the transition state are converted to so-called pentad intensities as obtained from ¹³C-NMR spectra of the polymer. From the pentad distribution it is possible to extract information about the configuration of five neighboring methyl groups along the polypropene backbone. Through Maxwell-Boltzmann statistics the calculated MM energies are converted to probabilities for obtaining each diastereomer, and in turn, to probabilities for sequences of such diastereomers. The intensity of a given pentad is finally obtained by considering all possible five-membered sequences contributing to that pentad.

For isopropylidene-bridged zirconocene catalysts such as [ⁱPr(3-X-CpFlu)}ZrR]⁺ (X=H, Me, Et, ⁱPr, ^tBu; Cp=cyclopentadienyl, Flu=fluorenyl), the computed pentad distributions generally follow the observed ones below 30–50°C, with typical RMS deviations for the 10 pentads of a given catalyst remaining within a few percentage-points. Above 30–50°C the observed decrease in specificity is generally underestimated by the calculations, indicating the onset of competing isomerization reactions at elevated temperatures.

The computational results⁴ indicate that the molecular structure of the catalyst cation is even more decisive to the polymer microstructure than previously assumed. The refined description of the catalyst–polymer relationship, especially the introduction of the effects of temperature, has also brought about new mechanistic insight, in particular regarding the role of intermediate chain migration (back-skip)³. Finally, accurate prediction of polymer microstructure from independent means also seems to be a strategy of potential value for catalyst development and improvement.

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Implementation of an NDDO/CI/SOS Approach for Second-Order Hyperpolarizabilities

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The sum-over-states (SOS) formalism implemented in VAMP [1] for NDDO-Hamiltonians AM1, PM3 and MNDO for the calculation of hyperpolarizabilities [2a, 2b] was extended to third-order nonlinear optical properties [2c] and its application to third harmonic generation (THG). Extensive comparisons between THG experimental data and published MOPAC/FF to VAMP/PECI/SOS and AMPAC/FF calculated values were carried out in gas phase and in solvent for a data set of 236 compounds of the general type D π A and conjugated π -systems. Great care was taken to derive the global minimum conformers yielding significant deviations of the geometries derived by the three Hamiltonians. The data set therefore gives an overview of the shortcomings and strenghtenesses of the semiempirical methods. Here, the implementations of solvent effects in both semiempirical packages especially are problematic in the case of elongated molecules, so a threshold for molecular globularity had to be defined to eliminate erroneous data. The presented correlation statistics for γ are in acceptable agreement for the whole data set as for all experimentally well-defined substance classes with scalable correlation slopes smaller than unity. The data become more reliable for large γ , probably due to more precise experimental values. Inclusion of solvent effects raises the polarizabilities of the molecules consistently. These results enable us to qualitatively predict trends for small as well as large second-order polarizabilities, derive scaling functions for quantitative predictions and calculate tensor elements of γ experimentally not accessible. The SOS formalism even allows us to obtain insights in frequency-dependence of second-order hyperpolarizability effects beyond THG.

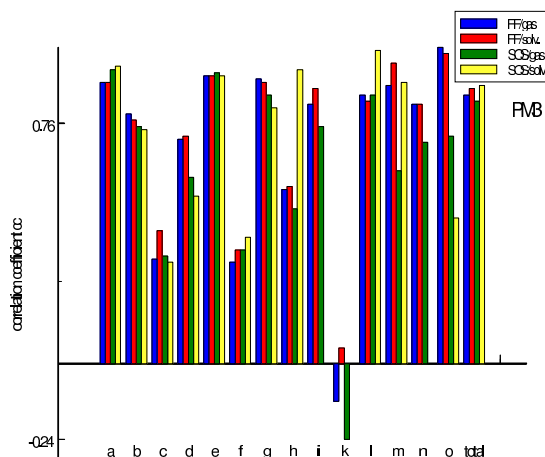


Figure 1: Experiment vs. calculation correlations for gas phase and solvent model derived $\langle\gamma\rangle$ with AMPAC/finite field and VAMP/CI/SOS methods for the different substance classes

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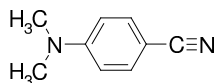
Ab Initio Calculations and Molecular Dynamics Simulations of Intramolecular Charge Transfer in 4-(N,N-Dimethylamino)benzonitrile

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DMABN

4-(N,N-Dimethylamino)benzonitrile (DMABN) is the prototype of a group of organic donor-acceptor compounds that can undergo intramolecular charge transfer (ICT) in the excited singlet state. In polar solvents, it exhibits dual fluorescence: Apart from “normal” emission out of the locally-excited (LE) state, which is also present in the gas phase and in nonpolar solvents, in polar solvents a second, “anomalous”, strongly red-shifted band is observed in the spectrum, attributed to a charge-transfer (CT) state [1]. This phenomenon has been mostly explained by the twisted ICT (TICT) mechanism [2], which claims that the electron transfer is induced by a rotation of the amino group around its bond to the benzene moiety. According to the wagged ICT (WICT) model [3], another possible source of charge separation is the pyramidalization of the amino nitrogen. Recently, a new concept for understanding the dual fluorescence, called rehybridized ICT (RICT) [4], which involves bending and stretching of the nitrile group, was proposed.

In the poster, we will present single-point calculations of CASPT2 potential-energy profiles and CASSCF dipole moments at CIS optimized geometries of isolated DMABN along the TICT, WICT and RICT reaction paths in the lowest excited singlet states [5]. All results appear to be strongly dependent on the amount of electron correlation included. Already in the Franck-Condon region a moderately polar L_b and a strongly polar L_a state are found with the L_b state lying below the L_a state. Twisting is the sole reaction coordinate that leads to an intersection of the two states and appropriate dipole-moment changes. Wagging causes only minor changes of the potential-energy profiles and dipole moments. Along the rehybridization reaction path, another CT state is strongly stabilized, but does not become the global singlet excited-state minimum.

Solvent effects along the TICT reaction path were examined by combining the CASPT2 potential energies and CASSCF atomic charges with molecular dynamics (MD) simulations in the solvents cyclopentane and acetonitrile [6]. Adiabatic potential-energy profiles and vertical energy gaps were evaluated using equilibrium MD simulations. Solvent effects in cyclopentane turn out to be negligible. In acetonitrile, the L_a state is shifted below the L_b state and develops a potential-energy minimum at the fully-twisted geometry. Fluorescence at this geometry is strongly red-shifted, mainly due to the increase of the ground-state energy upon twisting. The calculated vertical excitation energies are in good agreement with experiment, whereas the Stoke's shift in acetonitrile is underestimated by about 0.4 eV. The solvation dynamics in acetonitrile directly after absorption was investigated by nonequilibrium MD simulations. The solvent response is very rapid and consists of two parts, the major of which is completed within about 0.2 ps.

The present calculations support the TICT mechanism for the occurrence of dual fluorescence in DMABN in polar solvents.

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Dissipative quantum dynamics for laser induced desorption

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A new approach[1] to dissipative quantum dynamics shall be applied in the theoretical description of laser induced desorption of small molecules from metal oxide surfaces. Wave packet calculations on ab initio potential energy surfaces for the electronic ground state and a representative excited state have been performed for NO adsorbed on a NiO(100) surface[2, 3]. However, the finite lifetime of the excited state has been included only semi-empirically.

To treat the dissipative quantum dynamics rigorously, we employ the surrogate Hamiltonian theory[1]. The adsorbate/substrate complex is divided into the system and the environment. The bath consists of electron-hole-pairs in the surface which are described as two-level-systems. The adsorbate is coupled to the bath via a dipole-dipole-interaction and transitions between the ground and excited potential energy surfaces are induced by this coupling. A surrogate hamiltonian with a finite number of bath modes is constructed leading to a controllable approximation in which the necessary number of bath modes depends on the propagation time. The laser pulse exciting the adsorbate is included semiclassically. Thus the influence of different pulse lengths, intensities and shapes on the desorption as well as the interplay of dissipation and excitation can be investigated.

We present the method and first results.

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Towards a Catalyst for Alkene Hydroamination – Static and Dynamic *Ab Initio* DFT Studies

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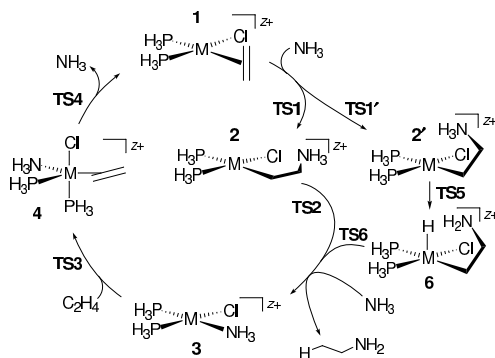
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Using density functional theory, we have investigated group 9 and group 10 d⁸ transition-metal complexes in view of their potential application as catalysts for the **hydroamination of alkenes** [1]. We used the **projector-augmented wave (PAW) method** [2], a plane-waves-based method with all-electron wavefunctions capable of performing **Car–Parrinello *ab initio* molecular dynamics** simulations.

Transition states were located using friction dynamics combined with a moving constraint to drive the system over the barrier, while all other degrees of freedom were being relaxed. Dynamical reaction paths were obtained by letting the system evolve freely from the transition state, thus allowing a detailed analysis of the time evolution of the reaction event [3].

The principal mechanistic pathway explored involves external nucleophilic attack of the amine on the coordinated alkene (C=C activation), followed by either protonolytic cleavage of the metal–alkyl bond or protonation of the metal with subsequent C–H reductive elimination. Complexes of the type {MCl(PH₃)₂}ⁿ⁺ have been studied, where M = Ni(II), Pd(II), Pt(II) (*n* = 1) or M = Co(I), Rh(I), Ir(I) (*n* = 0).

The reaction profiles for the complete catalytic cycle will be discussed, assessing the suitability of the metal complexes. The influence of ligand electronic effects on the rate-determining step has been investigated by replacing PH₃ by a series of substituted phosphanes PR₃ (R = F, CF₃, Me, NMe₂, Ph, *p*-C₆H₄OMe, *p*-C₆H₄NMe₂) with different electron-donating capabilities.



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Theoretical study of the dissociation of small neon clusters

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The Molecular Dynamics with Quantum Transitions method (MDQT) is applied to investigate the dynamics of the dissociation of small ionized neon clusters (up to 7 atoms). The motion of the neon atoms is treated classically, while transitions between the different potential energy surfaces (PES) of the ionic clusters are treated quantum mechanically. These PES are generated using the semiempirical diatomics-in-molecule method (DIM) applied to a minimal basis set consisting of the 2p orbitals of each neon atom, in addition the induced dipole-induced dipole interaction is taken into account.

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All-Electron Ab-Initio Molecular Dynamics

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We present an all-electron implementation of the Gaussian and Augmented-Plane-Wave density functional method (GAPW method), which allows ab-initio density functional calculations for periodic and non-periodic systems. The results of the all-electron calculations for a representative set of small molecules are reported to demonstrate the accuracy and reliability of the GAPW method. Furthermore, the performance of the GAPW method is shown for some larger molecules. Finally, as a first test an all-electron ab-initio molecular dynamics (MD) run was performed for 32 water molecules in a simple cubic box under ambient conditions.

Chemical Shift driven Molecular Dynamics and Structure Optimization

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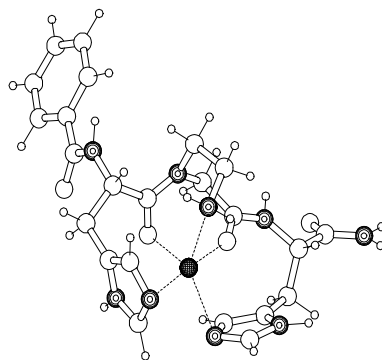
Common NMR measurements provide three kinds of structural information: J-coupling constants between nuclei separated by bonds which reflects the size of dihedral angles, nuclear Overhauser enhancement intensities corresponding to interproton distances and chemical shifts containing the whole nearby electronic structure information.

We represent a chemical shift driven molecular dynamics and geometry optimisation for structure investigation. This method needs energy gradients every step either during a molecular dynamics or a geometry optimisation. In order to calculate forces very fast a new developed universal force field with fluctuating charges is used. Additionally to the molecular force field correcting contributions, pseudo forces, due to chemical shift deviations of experimental and calculated values are introduced. Chemical shift values attributed to corresponding atoms are considered for correction. These pseudo forces need to be calculated every time step. Hence an effective method for obtaining theoretical chemical shifts of atoms are needed. For this we treat a semiempirical bond polarisation theory. In this theory the chemical shift depends on all other charged sites around. The chemical shift is proportional to the quantum chemical polarisation energies of all located bond orbitals (χ) due to surrounding charged sites (q). The formula for the isotropic chemical shift (σ) is given as:

$$\sigma_a = \sum_i \left(\delta_{ab_i}^0 + \delta_{ab_i}^1 \sum_x \left(\left\langle \chi_{a_i} \left| \frac{q_x}{R_{a_i,x} - r} \right| \chi_{a_i} \right\rangle - \left\langle \chi_{b_i} \left| \frac{q_x}{R_{b_i,x} - r} \right| \chi_{b_i} \right\rangle \right) \right)$$

The proportionality factors (δ^0 , δ^1) are obtained for ^{13}C bonded to Hydrogen, Oxygen and Nitrogen.

We represent a ^{13}C chemical shift structure investigation on the pseudo peptide Bz-His-(N-CH₂-CH₂-NH₂)Gly-His-NH₂ and its Zn-complex:



Quantum Dynamical Investigation of Photochemical Reactions Beyond the Born Oppenheimer Approximation

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We focus on the quantum mechanical and quantum dynamical description of photochemical reactions, where we are interested in ultrafast chemical reactions mediated by conical intersections (Colns) as well as on the manipulation of chemical processes by means of optimally designed ultrashort laser pulses.

As model system for electrocyclic reactions that occur on the femtosecond timescale, we study the lightinduced ringopening of cyclohexadiene (CHD). To do so, we reduce the highdimensional (36) system to sufficiently few reactive coordinates that are relevant for the description of its ultrafast dynamics. With the help of those we derive ab initio potential energy surfaces, which are then used in our quantum dynamical simulations.

In the CHD/hexatriene system at least two Colns S_1/S_0 are energetically reachable and can be accessed with different branching ratios by varying the initial wavepacket. Results of this “passive” control are presented and we hope to extend our investigations on this molecule to “active” control schemes such as optimal control theory (OCT).

To relate our results and interpretations to a description within a normal mode picture, we derive a formalism that enables us to project the molecules motion in the reactive coordinate space onto its normal modes. This not only provides insight in the validity of a normal mode description in the context of Colns but can also be a starting point to directly compare our results to an experiment.

Of high practical relevance in radical chain reactions is acetylen. Herein experimentalists would like to selectively prepare vibrational states to demonstrate the potency of a new chemistry with laserlight.

To attack the preparation problem we reduce the molecule’s Hamiltonian to the experimentally interesting vibrational modes, which in this case are IR-active. Analysis of the electron density’s change during these vibrations indicates highest reactivity when exciting the asymmetric CH-stretch mode.

For distinct populations of the IR-active modes we compute the corresponding potential energy surface and eigenfunctions and then use OCT strategies to calculate laser pulses that can be applicable in an experiment for a state selective preparation of acetylen.

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Parallelization of the Dirac-Fock package MOLFDIR: A pathway for the treatment of large relativistic systems

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The treatment of relativity and electron correlation on an equal footing is essential for the computation of systems containing heavy elements. Even if there are several reliable approximations to the Dirac-Fock equation mostly based on reduction to fewer components of the wave function full Dirac-Fock calculations will provide the most accurate way for taking relativity into account. Since the treatment of electron correlation is already a very demanding task in nonrelativistic calculations the memory and disk space requirements grow much bigger when the wave function has four components. Especially the integral generation and the corresponding transformation from the AO to the MO basis need a lot of computer resources. For larger systems the enormous memory and disk space requirements can only be handled by a parallel approach to the problem. Here we present the parallelization of the program package MOLFDIR up to the four-index transformation step. A parallelization of the CCSD(T) code is necessary when the active space becomes very large but in the case of large basis sets and moderately large active spaces the parallelization of the CCSD(T) code is not urgent and will be done later on. The integral calculation, the SCF part and four-index transformation are fully parallelized whereas the one-electron integrals and their transformation can be performed on each node separately or on one node with a subsequent distribution of the corresponding files depending on the computer architecture. The current implementation is based on a distributed memory system since these architectures can be easily enlarged and are cheaper than shared memory machines. Since communication is a bottleneck on these systems large data transfer has to be avoided. We therefore generate the two-electron integrals in a way that makes it possible to keep the four-index transformation independent from the other nodes up to the very last step where the MO contributions are added up. Calculations on a test system show the scaling properties of the code up to the transformation step.

THE ALL-ELECTRON TREATING OF THE SPIN-ORBIT INTERACTION BASED ON SINGLE-DETERMINANT WAVEFUNCTION

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Two possible approaches for treating the spin-orbit effects in heavy element systems are presented here: a) The double-perturbative treatment at the post-HF level together with the electron correlation, b) The variational two-component approach where the spin-orbit term is added to the scalar Hamiltonian and the energy functional is minimized. The former is proposed for calculating the spin-orbit energy shift in closed-shell systems, the latter is suitable also for calculating the spin-orbit splitting in open-shell systems. In both approaches the effective one-electron (mean-field) spin-orbit operator is used.

Perturbation theory of magnetic properties and relativistic corrections based on the Lévy-Leblond equation

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Abstract

Starting from the Lévy-Leblond equation, which is the four-component non-relativistic limit of the Dirac equation, a direct perturbation theory of magnetic properties and relativistic corrections is formulated. Furthermore, operators and matrix elements are derived that occur when the nuclei of the molecule are described by Gaussian charge distributions and Gaussian magnetic dipole distributions instead of point charges and magnetic point dipoles.

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Polarized atomic orbitals for linear scaling methods

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We present a modified version of the polarized atomic orbital (PAO) method of Lee and Head-Gordon [1] to construct minimal basis sets optimized in the molecular environment. The minimal basis set derives its flexibility from the fact that it is formed from atom-centered linear combinations of a larger set of atomic orbitals. This approach significantly reduces the number of independent variables that are to be determined during a calculation, while retaining most of the essential chemistry resulting from the admixture of higher angular momentum functions.

Furthermore, we combine the PAO method with linear scaling algorithms. We use the Chebyshev polynomial expansion method of Goedecker and Teter [2] and the canonical purification of the density matrix developed by Palser and Manolopoulos [3]. This scheme seems to overcome one of the major drawbacks of standard approaches for large nonorthogonal basis sets, namely numerical instabilities resulting from ill-conditioned overlap matrices. We find that the condition number of the PAO overlap matrix is independent from the condition number of the underlying extended basis set and consequently no numerical instabilities are encountered.

Various applications are shown to confirm this conclusion and to compare the performance of the PAO method against extended basis set calculations.

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Linear Response CCSD triplet excitation energies using an explicit spin-coupling.

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Abstract

An atomic-integral direct linear response coupled cluster singles and doubles (CCSD) model to calculate triplet excitation energies is presented. The excitation space is parametrized in terms of excitation operators that are explicit coupled to triplet spin.

The triplet excitation spectrum of benzen is calculated in a basis ranging from 147 to 432 basisfunctions. The calculated triplet excitation energies are compared with experimental and other theoretical values.

Preliminary results will be presented for porphin with up to 678 basisfunctions.

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