

International Meeting on Atomic and Molecular Physics and Chemistry

CSIC, Madrid (Spain)
June 29 – July 2 (2010)



Book of Abstracts

Welcome to Madrid and welcome to the International Meeting on Atomic and Molecular Physics and Chemistry - IMAMPC 2010.

This conference has been conceived to give the opportunity to as many young researchers as possible to present the results of their recent investigations on a broad spectrum of different subjects such as Molecular Electronic Structure at the Gas Phase and Gas/Surface Interface, Macromolecules and Aggregates, Structural Dynamics, Liquids, Nanomaterials, Bose-Einstein Condensation, Biophysics and Biochemistry, Photoreactivity, Molecular Dynamics, Atomic and Molecular Collisions, Reactive and Ultra-Cold Collisions, or Quantum Control.

The organization of the event has been only possible with the coordinated work of five researchers; definitely the result of a team effort. Our attempts to organize this event in the most efficient manner have always been accompanied with the support of our Department (Física Atómica, Molecular y de Agregados) and Institute (Instituto de Física Fundamental). It is therefore a pleasure to acknowledge such a confidence in our initiative. We do not want to forget either the list of contributing sponsors which helped us to make this IMAMPC 2010 conference possible.

In this first edition, we will count on with participants from about 15 different countries. This pioneer idea of bringing together those who constitute the present and the short term future in our field, is intended to have a continuation in next editions in any of the countries which contribute this year in Madrid. One of our goals is to convince you to host the next IMAMPC conference. You will have all our support and experience to help with you in that duty.

We would be very pleased if we manage you to feel comfortable with us in Madrid and to enjoy a fruitful and friendly meeting.

THE ORGANIZERS:

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Index

<i>Program</i>	7
<i>Talks</i>	15
<i>Oral Contributions</i>	63
<i>Posters</i>	75
<i>List of Participants</i>	105

Program

Tuesday, June 29

15:00-16:00

Registration

16:00-16:15

Welcome reception – Opening session

16:15-18:35

Session Tu1 (Chair: *Franco A. Gianturco*)

16:15-16:40 E. Martínez Nuñez : *Chemical dynamics simulations of Ar, CO₂ and NO scattering from a perfluorinated self-assembled monolayer surface*

16:40-17:05 N. Sändig : *Adsorption, motion and viscosity of organic molecules on gold*

17:05-17:30 L. M. Molina : *Ab initio studies of propene epoxidation at noble metal nanocatalysts*

17:30-17:55 S. Díaz Tendero : *Interferences between resonances localized in metal nanostructures supported on metal surfaces*

17:55-18:20 P. Jelinek : *Understanding of relation between chemical force and current at atomic scale*

18:20-18:35 Y. Wang : *Theoretical study on self-assembly of TCNQ adsorbed on Cu(100) surface*

Wednesday, June 30

9:15-10:45

Session W1 (Chair: *Octavio Roncero*)

- 9:15-9:40 L. Bonnet : *Classical reactive scattering in a quantum spirit*
9:40-10:05 F. Dayou : *Nonadiabatic dynamics on O_2+O_2 collisions*
10:05-10:30 P. Larrégaray : *Rationalizing the $S(^1D)+H_2$ cold reaction dynamics using a simple semiclassical statistical model*
10:30-10:45 M. Lara : *Reaching the cold regime: $S(^1D)+H_2$ open shell reactive collisions and the role of long-range interactions*
-

10:45-11:15

Coffee Break

11:15-12:30

Session W2 (Chair: *Pablo Villarreal*)

- 11:15-11:40 A. Nogales : *Relaxation behaviour in nanorods and nanotubes of PVDF and PVDF based ferroelectric polymers*
11:40-12:05 J. Ramos : *Simulation of folding processes of single-chain copolymers dilute solutions containing short chain branches*
12:05-12:30 S. Fernández-Alberti : *Excited state nonadiabatic molecular dynamics: energy funneling in light harvesting dendrimers*
-

12:30-13:30

Lunch

14:00-15:55

Session W3 (Chair: *José Campos Martínez*)

- 14:00-14:25 S. Cassasa : *CRYSCOR, a computational tool for the study of electronic correlation in crystals: Features and applications*
14:25-14:50 N. Lathiotakis : *Approximating electronic correlations with reduced density matrix functional*
14:50-15:15 B. González Landín : *Genetic algorithms search methods and applications in molecular clusters*
15:15-15:40 S. Stamatiadis : *Automatic differentiation via operator overloading: A Fortran 95 implementation*
15:40-15:55 S. López-López : *High-dimensional system-bath quantum dynamics with selected configurations wave functions*

15:55-16:25

Coffee Break

16:25-18:10

Session W4 (Chair: *Keneth C. Janda*)

- 16:25-16:50 G. Amaral : *Velocity map imaging in photodissociation of molecules: real time and energy resolved experiments*
- 16:50-17:15 R. Cireasa : *Real time imaging of ultrafast molecular dynamics*
- 17:15-17:40 E. González Noya: *The stability of a crystal with diamond structure for patchy particles with tetrahedral symmetry*
- 17:40-17:55 Á. Valdés : *Translation-rotation energy levels of one H₂ molecule inside the small and medium cages of the structure H clathrate hydrate*
- 17:55-18:10 R. Pérez de Tudela : *Path-integral Monte Carlo on atomic clusters*
-

18:10-18:45

Poster Presentation (Chair: *Jesús Rubayo Soneira*)

18:45-19:45

Poster Session – Wine Reception

Thursday, July 1

9:15-10:45

Session Th1 (Chair: *Marta I. Hernández*)

- 9:15-9:40 J. Aldegunde: *Hyperfine interactions in ultracold alkali dimers*
9:40-10:05 M. Rodríguez : *Periodic driving of ultracold atoms in optical lattices*
10:05-10:30 A. Simoni : *Ultracold atom-ion collisions: Landau quantization and scattering resonances*
10:30-10:45 J. M. Oldham : *Cold state-selective ion-molecule reactions*
-

10:45-11:15

Coffee Break

11:15-12:30

Session Th2 (Chair: *Gerardo Delgado-Barrio*)

- 11:15-11:40 G. M. Bruun : *Clock shifts in a Fermi gas interacting with a minority component: A soluble model*
11:40-12:05 I. Rabadán : *Isotope effects in ion-atom collisions*
12:05-12:30 D. de Fazio : *The hyperquantization algorithm: perspective of ab-initio quantum reactive scattering calculations*
-

12:30-13:30

Lunch

14:00-15:55

Session Th3 (Chair: *Fernando Flores*)

- 14:00-14:25 A. O. Mitrushchenkov : *Electric and elastic properties of wurtzite nanowires*
14:25-14:50 J. Ortega : *Analysis of the formation of metal/organic interfaces and nanocontacts using Density Functional Theory*
14:50-15:15 V. Timón : *Electronic bandstructure DFT analysis of metal cations substituted in phyllosilicates*
15:15-15:40 J. I. Martínez : *Trends in metal oxide stability for nanorods, nanotubes and surfaces*
15:40-15:55 S. Monturet : *Electronic structure and dynamics of the vibrational relaxation of NO molecules scattered of a gold surface*
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15:55-16:25 Coffee Break

16:25-18:10 Session Th4 (Chair: *Alberto García-Vela*)

- 16:25-16:50 A. Lombardi : *Oriented collision dynamics of simple chiral molecules*
- 16:50-17:15 J. Fernández-Castillo : *Ab initio potential energy surface and quasiclassical trajectory studies of the Cl+O₃ reaction*
- 17:15-17:40 C. Leonard : *Theoretical study of the predissociation of the A ²Π states of ZnF incorporating quasi-diabatization of the spin-orbit coupling*
- 17:40-17:55 A. Zanchet : *H₂ reactivity on gold clusters*
- 17:55-18:10 W. Unn-Toc : *Quantum dynamics at helium droplets*
-

21:00-23:00 Conference Dinner

Friday, July 2

9:15-10:45 Session F1 (Chair: Ramón Hernández Lamonedá)

- 9:15-9:40 C. Puzzarini : *Molecular structure determination: A testing ground for high level quantum-chemical computations*
- 9:40-10:05 A. Kalemós : *On the bonding interpretation of H₂SO₄, HNO₃, HClO₄ and O₃*
- 10:05-10:30 M. Biczysko : *Non-covalent interactions in the gas phase: new insights from experimental and computational spectroscopy*
- 10:30-10:45 C. Sanz : *Dynamic Stark control of the photodissociation of IBr molecule*
-

10:45-11:15 Coffee Break

11:15-12:30 Session F2 (Chair: Fernando Martín)

- 11:15-11:40 L. González : *Strong field effects in halomethanes*
- 11:40-12:05 I. Sola : *Laser driven bond lengths with parabolic chirped pulses*
- 12:05-12:30 B. Pons : *Self-consistent Bohmian description of laser-atom interactions*
-

12:30-13:30 Lunch

14:00-15:55 Session F3 (Chair: Salvador Miret Artés)

- 14:00-14:25 R. de Nalda : *Molecular videos: watching chemical change with ultrashort lasers*
- 14:25-14:50 A. S. Sanz : *Bohmian mechanics: A novel tool to explore the physics and chemistry of atoms and molecules*
- 14:50-15:15 B. Maté : *A study of CH₄/H₂O ices by infrared spectroscopy*
- 15:15-15:40 G. Fanourgakis : *A fast path integral method for polarizable force fields. Application to liquid water and ice*
- 15:40-15:55 J. S. Medina : *Molecular dynamics simulations of liquid water models: Temperature dependence of viscosities*
-

16:00-16:30 Coffee Break

16:30-18:25

Session F4 (Chair: Luis Bañares)

- 16:25-16:50 R. Z. Martínez : *Simulated Raman spectroscopy for the study of collisional energy transfer: Determination of rotational state-to-state relaxation rates in acetylene*
- 16:50-17:15 P. O’Keeffe : *Velocity map imaging of photoelectrons in a pump-probe experiments combinig synchrotron and laser radiation*
- 17:15-17:40 N. Gidopoulos : *Quantum mechanical description of vibrations in molecules and solids*
- 17:40-17:55 D. López-Durán : *ASPIN: An all spin scattering code*
- 17:55-18:10 P. Bargeño : *Subcritical temperature in Bose-Einstein condensates of chiral molecules*
-

18:10-18:30

Conclusions

21:00-22:00

Guided Tour (Madrid)

Talks

List of Talks

- J. Aldegunde:** *"Hyperfine interactions in ultracold alkali dimers"*
- G. Amaral:** *"Velocity map imaging in photodissociation of molecules: real time and energy resolved experiments"*
- M. Biczysko:** *"Non-covalent interactions in the gas phase: new insights from experimental and computational spectroscopy"*
- L. Bonnet:** *"Classical reactive scattering in a quantum spirit"*
- G. M. Bruun:** *"Clock shifts in a Fermi gas interacting with a minority component: A soluble model"*
- S. Cassasa:** *"CRYSCOR, a computational tool for the study of electronic correlation in crystals: Features and applications"*
- R. Cireasa:** *"Real time imaging of ultrafast molecular dynamics"*
- F. Dayou:** *"Nonadiabatic dynamics on O_2+O_2 collisions"*
- D. de Fazio:** *"The hyperquantization algorithm: perspective of ab-initio quantum reactive scattering calculations"*
- R. de Nalda:** *"Molecular videos: watching chemical change with ultrashort lasers"*
- S. Díaz Tendero:** *"Interferences between resonances localized in metal nanostructures supported on metal surfaces"*
- A. S. Sanz:** *"Bohmian mechanics: A novel tool to explore the physics and chemistry of atoms and molecules"*
- G. Fanourgakis:** *"A fast path integral method for polarizable force fields. Application to liquid water and ice"*
- S. Fernández Alberti:** *"Excited state nonadiabatic molecular dynamics: energy funneling in light harvesting dendrimers"*
- J. Fernández Castillo:** *"Ab initio potential energy surface and quasiclassical trajectory studies of the $Cl+O_3$ reaction"*
- N. Gidopoulos:** *"Quantum mechanical description of vibrations in molecules and solids"*
- B. González Landín:** *"Genetic algorithms search methods and applications in molecular clusters"*
- L. González:** *"Strong field effects in halomethanes"*
- E. González Noya:** *"The stability of a crystal with diamond structure for patchy particles with tetrahedral symmetry"*
- P. Jelinek:** *"Understanding of relation between chemical force and current at atomic scale"*
- A. Kalemou:** *"On the bonding interpretation of H_2SO_4 , HNO_3 , $HClO_4$ and O_3 "*
- P. Larrégaray:** *"Rationalizing the $S(^1D)+H_2$ cold reaction dynamics using a simple semi-classical statistical model"*
- N. N. Lathiotakis:** *"Approximating electronic correlations with reduced density matrix functional"*
- C. Leonard:** *"Theoretical study of the predissociation of the $A^2\Pi$ states of ZnF incorporating quasi-diabatization of the spin-orbit coupling"*
- A. Lombardi:** *"Oriented collision dynamics of simple chiral molecules"*
- J. I. Martínez:** *"Trends in metal oxide stability for nanorods, nanotubes and surfaces"*
- E. Martínez Nuñez:** *"Chemical dynamics simulations of Ar, CO_2 and NO scattering from a perfluorinated self-assembled monolayer surface"*

R. Z. Martínez Torres: *“Simulated Raman spectroscopy for the study of collisional energy transfer: Determination of rotational state-to-state relaxation rates in acetylene”*

B. Maté: *“A study of CH₄/H₂O ices by infrared spectroscopy”*

A. O. Mitrushchenkov: *“Electric and elastic properties of wurtzite nanowires”*

L. M. Molina: *“Ab initio studies of propene epoxidation at noble metal nanocatalysts”*

A. Nogales: *“Relaxation behaviour in nanorods and nanotubes of PVDF and PVDF based ferroelectric polymers”*

P. O’Keeffe: *“Velocity map imaging of photoelectrons in a pump-probe experiments combining synchrotron and laser radiation”*

J. Ortega Mateo: *“Analysis of the formation of metal/organic interfaces and nanocontacts using Density Functional Theory”*

B. Pons: *“Self-consistent Bohmian description of laser-atom interactions”*

C. Puzzarini: *“Molecular structure determination: A testing ground for high level quantum-chemical computations”*

I. Rabadán: *“Isotope effects in ion-atom collisions”*

J. Ramos: *“Simulation of folding processes of single-chain copolymers dilute solutions containing short chain branches”*

M. Rodríguez: *“Periodic driving of ultracold atoms in optical lattices”*

N. Sändig: *“Adsorption, motion and viscosity of organic molecules on gold”*

A. Simoni: *“Ultracold atom-ion collisions: Landau quantization and scattering resonances”*

I. Sola Reija: *“Laser driven bond lengths with parabolic chirped pulses”*

S. Stamatidis: *“Automatic differentiation via operator overloading: A Fortran 95 implementation”*

V. Timón: *“Electronic bandstructure DFT analysis of metal cations substituted in phyllosilicates”*

Hyperfine interactions in ultracold alkali dimers

Jesús Aldegunde^(a)

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We have investigated how the hyperfine interactions affect basic properties (energy levels and microwave spectra) of homo- and heteronuclear alkali-metal dimers in levels correlating with the lower rotational states of the ground electronic state^{1,2}. The results are crucial in efforts to produce ground-state ultracold molecules and for their subsequent applications. As an example, we show how the explicit consideration of the hyperfine splittings will influence the design of quantum computing implementations involving ultracold alkali dimers^{3,4}.

¹ J. Aldegunde, Ben A. Rivington, Piotr S. Zuchowski and Jeremy M. Hutson, *Phys. Rev. A* **78**, 033434 (2008)

² J. Aldegunde and Jeremy M. Hutson, *Phys. Rev. A* **79**, 013401 (2009)

³ J. Aldegunde, Hong Ran and Jeremy M. Hutson, *Phys. Rev. A* **80**, 1 (2009)

⁴ Hong Ran, J. Aldegunde and Jeremy M. Hutson, *New. J. Phys.*, [arXiv:0909.3644](https://arxiv.org/abs/0909.3644)

VELOCITY MAP IMAGING in photodissociation of molecules: real time and energy resolved experiments.

G.A. Amaral^(a)

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The velocity map imaging (VMI) technique is a powerful tool which coupled to nanosecond and/or femtosecond lasers provides complete information of a photodissociation event. Upon absorption of energy in the form of light, molecules are promoted to an unstable excited state which can deactivate by breaking bonds forming two or more fragments.

If the energy source is a pulsed nanosecond laser beam (pulse duration of up to 10 ns), the technique is applied to measure the energy partitioning between fragments. This, in turn, is a reflection of the pathway involved in the process of bond breaking allowing the characterization of the mechanism and the potential energy surfaces involved. This technique has been successfully employed in our lab to resolve the photodissociation of CH₃I in the red edge of its first absorption band (A)¹ as well as in the exploration of the newly discovered roaming mechanism in CH₃CHO photodissociation^{2,3}.

If, on the other hand, the energy source is a pulsed femtosecond laser beam (pulse duration of up to 60 fs), the technique is used to measure the time evolution of the bond breaking process. This means that an actual clocking of the reaction process can be performed where the time that it takes for the bond to break is precisely measured. Furthermore, transient species which only exist briefly as the reaction progresses from reactants to products can be detected and even characterized. This technique has been applied in our lab to the time characterization of the photodissociation of CH₃I in its first absorption band (A)⁴. In the present talk the most relevant aspects of both types of VMI experiments will be introduced. The main results of the experiments mentioned above will be presented and discussed as well as some future applications for this powerful and versatile technique.

Non-covalent interactions in the gas phase: new insights from experimental and computational spectroscopy

M. Biczysko^(a,b), J. Bloino^(a,b) and V. Barone^(b)

^(a) *Dipartimento di Chimica "Paolo Corradini", Università Federico II di Napoli and INSTM-UdR Napoli, Via Cintia, 80126 Napoli, Italy*

^(b) *Scuola Normale Superiore, Piazza dei Cavalieri 7, 56126 Pisa, Italy*

Recently, many gas phase spectroscopic studies have been focused on the understanding of the nature of weak interactions in model biological systems and microsolvation phenomena. However, only few of them have been performed under high-resolution conditions. Among the aromatic molecules, anisole is particularly interesting due to the possibility of different solvent-molecule interaction schemes: hydrogen bonding, van der Waals forces, dipole-dipole interactions.

The study of the non-covalent interactions in dimers of anisole has taken full advantage of the versatile method we developed to compute vibrationally resolved electronic spectra from first principles [1,2]. The integrated procedure has first been exploited to simulate the gas phase optical spectra of the $S_1 \leftarrow S_0$ electronic transitions of anisole. On the whole, a remarkable agreement between computed and experimental vibrationally resolved REMPI spectrum has been achieved [3], allowing for the revision of some assignments of fundamental vibrations in the S_1 state of anisole. Next, the results from high resolution spectroscopic observations combined with computational studies led to the unequivocal determination of the ground and excited state stacking equilibrium structures of the anisole dimer [4]. Moreover, the direct comparison between theoretical vibrationally resolved electronic spectra and experimental REMPI spectra of clusters with different isotopic composition revealed the local excitation character for the $S_1 \leftarrow S_0$ electronic transition [5]. The overall combined experimental/theoretical study permitted a detailed description of the stacking interaction in the anisole dimer.

¹ V. Barone, J. Bloino, M. Biczysko, F. Santoro *J. Chem. Theory Comput.* **5**, 540 (2009)

² J. Bloino, M. Biczysko, F. Santoro, V. Barone *J. Chem. Theory Comput.* **6**, 1256 (2010)

³ J. Bloino, M. Biczysko, O. Crescenzi, V. Barone *J. Chem. Phys.* **128**, 244105 (2008)

⁴ G. Pietraperzia, M. Pasquini, N. Schiccheri, G. Piani, M. Becucci, E. Castellucci, M. Biczysko, J. Bloino, V. Barone *J. Phys. Chem. A* **113**, 14343 (2009)

⁵ N. Schiccheri, M. Pasquini, G. Piani, G. Pietraperzia, M. Becucci, M. Biczysko, J. Bloino, V. Barone *Phys. Chem. Chem. Phys.* Submitted

Classical Reactive Scattering in a Quantum Spirit

L. Bonnet

*Institut des Sciences Moléculaires, Université Bordeaux I,
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The goal of the talk is to show how the quasi-classical trajectory (QCT) approach of chemical reaction dynamics can be improved by adding quantum constraints in the light of the semiclassical description of molecular collisions.

Two additions are considered; first, trajectories do not carry the same statistical weight, like in the traditional QCT method. Instead, they carry a Gaussian weight such that the closer the final vibrational actions to integer values, the larger the weight [1-5]. Second, vibrationally adiabatic non reactive trajectories are omitted in the calculation of final attributes [4].

For polyatomic reactions, however, the use of Gaussian weights (GW) may be problematic, as the number of trajectories to be performed dramatically increases with the number of vibrational degrees-of-freedom. In the case of indirect photodissociations, the statistico-dynamical approach represents an interesting alternative the application of which is made easier by a transformation from action-angle to Cartesian coordinates [6,7].

The validity of the resulting treatments is checked by comparing their predictions with those of exact quantum scattering approaches or experimental results.

- [1] L. Bonnet and J.-C. Rayez, *Chem. Phys. Lett.*, 277, 183 (1997).
- [2] L. Banares, F. J. Aoiz, P. Honvault, B. Bussery-Honvault and J.-M. Launay, *J. Chem. Phys.*, 118, 565 (2003).
- [3] L. Bonnet and J.-C. Rayez, *Chem. Phys. Lett.*, 397, 106 (2004).
- [4] L. Bonnet, *J. Chem. Phys.*, 128, 044109 (2008).
- [5] L. Bonnet, *Chin. J. Chem. Phys.*, 22, 210 (2009).
- [6] M. L. Gonzalez-Martinez, L. Bonnet, P. Larrégaray, J.-C. Rayez and J. Rubayo-Soneira, *J. Chem. Phys.*, 130, 114103 (2009).
- [7] M. L. Gonzalez-Martinez, L. Bonnet, P. Larrégaray and J.-C. Rayez, *Phys. Chem. Chem. Phys.*, 12, 115 (2010).

Clock shifts in a Fermi gas interacting with a minority component: a soluble model

G. M. Bruun
*CELIA, Univ. of Copenhagen – Niels Bohr Inst.
Denmark*

We consider the absorption spectrum of a Fermi gas mixed with a minority species when majority fermions are transferred to another internal state by an external probe. In the limit when the minority species is much more massive than the majority one, we show that the minority species may be treated as static impurities and the problem can be solved in closed form. The analytical results bring out the importance of vertex corrections, which change qualitatively the nature of the absorption spectrum. It is demonstrated that large line shifts are not associated with resonant interactions in general. We also show that the commonly used ladder approximation fails when the majority component is degenerate for large mass ratios between the minority and majority species and that bubble diagrams, which correspond to the creation of many particle-hole pairs, must be taken into account. We carry out detailed numerical calculations, which confirm the analytical insights and we point out the connection to shadowing phenomena in nuclear physics.

¹ G. M. Bruun, C. J. Pethick and Z. Yu, *Phys. Rev. A* **81**, 033621 (2010).

CRYSCOR, a computational tool for the study of electronic correlation in crystals: features and applications

S. Casassa, L. Maschio, M. Halo, A. Erba and C. Pisani^(a)
(a) *Dipartimento di Chimica I.F.M., Università di Torino, Turin, Italy.*

CRYSCOR is a post-Hartree-Fock (HF) local correlation program for non conducting crystals¹. The reference HF solution, on top of which the Møller-Plesset perturbative method at the second order (MP2) is implemented, is provided by CRYSTAL². Well-localized symmetry-adapted Wannier functions are adopted to describe the occupied manifold: this permits the exploitation of the short-range nature of electron correlation, following the general scheme of Pulay³.

The original features due to the extension of the local approach to periodic systems are presented⁴ and CRYSCOR's capabilities, its range of validity and its present limits are discussed with the help of some test cases. Finally, some applications are illustrated (physisorption of small molecules on oxide surfaces; methane clathrate; molecular crystals) and further developments envisaged.

¹ www.cryscor.unito.it

² www.crystal.unito.it

³ P. Pulay *Chem. Phys. Lett.* **100**, 151 (1983); S. Szabo and P. Pulay *Chem. Phys. Lett.* **113**, 13 (1985)

⁴ L. Maschio, D. Usvyat, C. Pisani, F. Manby, S. Casassa and M. Schütz *Phys. Rev. B* **76**, 075101 (2007)

Real time imaging of ultrafast molecular dynamics

R. Cireasa, V. Blanchet and N. Thiré

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The advent of the Velocity Map Imaging has revolutionised the experimental approaches used in the molecular dynamics studies as it offers a multiplex detection method, which provides exceptional energy resolution alongside with simultaneous measurements of the angular distributions. Ever since its introduction in the late 1990s, this powerful technique has underpinned significant advances in our understanding of atomic and molecular processes and it has been applied to numerous studies of fundamental dynamical processes: bimolecular collisions, photodissociation and photoionisation. In combination with time resolved measurements, the ion and photoelectron imaging sheds light onto the pathways followed by the molecules from the entrance to the exit channel. Imaging with femtosecond resolution produces the 'movie' of the molecular transformation by giving real time information on the electronic and nuclear wave-packet motions, electronic dephasing, and photoionization and photodissociation dynamics.

We will illustrate the potential of the imaging method for the study of complex and fast dynamics through our results obtained for the study of two benchmark systems: CH₃I and NO₂. For the former, we will discuss the photionisation and the predissociation of CH₃I (6s) *B*(²E) Rydberg state initiated around 200 nm. As for NO₂, we will present the results obtained for the study of the competing multiphoton and multichannel dynamics induced with femtosecond pulses of 400 and 266 nm.

Nonadiabatic dynamics in O₂+O₂ collisions

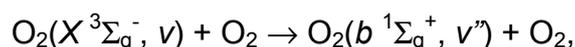
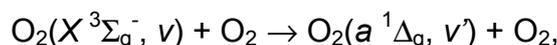
F. Dayou^(a), M.I. Hernández^(b), J. Campos-Martínez^(b) and R. Hernández-Lamoneda^(c)

^(a) *Laboratoire d'Etude du Rayonnement et de la Matière en Astrophysique, Observatoire de Paris-Meudon, Université Pierre et Marie Curie, Meudon Cedex 92195, France*

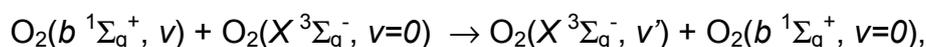
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The energy transfer by collisions involving the ground and excited species of molecular oxygen plays a crucial role in the chemistry of the upper Earth's atmosphere. The specificities of molecular oxygen (a stable radical in its ground $X^3\Sigma_g^-$ state, with two low-lying excited states $a^1\Delta_g$ and $b^1\Sigma_g^+$) provide appropriate conditions for a rich variety of collision-induced energy transfer mechanisms. Experimentally, the rate coefficients measured for the collisional removal of $O_2(X^3\Sigma_g^-, \text{high-}v)$, $O_2(a^1\Delta_g, \text{low-}v)$ and $O_2(b^1\Sigma_g^+, \text{low-}v)$ by O_2 are fast and show peculiar features which cannot be explained by simple vibrational cascading. The strong changes observed in the rate coefficients between adjacent vibrational levels suggest that near-resonant processes, involving electronic energy transfers, should dominate the removal processes. However, the final state distribution could not be probed experimentally, and theoretical studies are needed to unveil the underlying mechanisms. By resorting to a reduced dimensionality model of the dimer, together with *ab initio* methods and quantum dynamics calculations, we have shown¹ that *intra*-molecular electronic energy transfers,



mediated by spin-orbit couplings between the dimer states, were able to mimic the sharp changes observed in the measured collisional removal rate coefficients for $O_2(X^3\Sigma_g^-, v \geq 26)$. In a recent study², we have also addressed the problem of *inter*-molecular electronic energy transfer,



mediated by nonadiabatic radial couplings between the dimer states. It is found that the multidimensional nonadiabatic couplings can be predicted with high accuracy, compared to the *ab initio* results, by using analytical forms only depending on a reduced set of adiabatic energy terms. The results of quantum dynamics calculations for the removal of $O_2(b^1\Sigma_g^+, v \leq 3)$ are found qualitatively consistent with the experimental observations.

¹ F. Dayou, M.I. Hernández, J. Campos-Martínez and R. Hernández-Lamoneda, *J. Chem. Phys.* **126**, 194309 (2007)

² F. Dayou, M.I. Hernández, J. Campos-Martínez and R. Hernández-Lamoneda, *J. Chem. Phys.* **132**, 044313 (2010)

The hyperquantization algorithm: perspective of ab initio quantum reactive scattering calculations

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In the last thirty years, the fast increase of the computer resources available has permitted to achieve important results in computational sciences.

Early developments of the computer technology have increased the processor speed clock leading to always more efficient machines. Nowadays, due to physical limits, the processor speed clock cannot be increased further. However, the overall computer power still continues to increase quadratically thanks to the advent of multi-core chips that have permitted to build processors with an high number of computational cores. Parallel supercomputers with hundred thousands cores and several Terabytes of RAM memory are today available to the scientific community. These machines, if opportunely exploited, will drive a jump of order of magnitude on the size of feasible scientific problem to be treated. To efficiently exploit the new hardware resources, the computational algorithms must be massively parallelized taking into account the different speed of intra or inter node communications and mixing shared and distributed memory paradigms. The level of parallelizability is strictly dependent from the algebraic nature of the algorithm as well as from the quality of the parallelization strategy.

In this presentation I will illustrate the properties of the Hyperquantization Algorithm¹ that permit a very efficient parallelization of the reactive scattering code with very large speed-up on all the computational cores available on nowadays supercomputers. Particularly promising are the performances for calculations of ion-molecular systems at thermal energies as well as under cold and ultra-cold conditions where the coupling between mathematical properties of the Hyperquantization algorithm and parallelization open new perspectives for ab-initio quantum reactive scattering calculations.

¹ V. Aquilanti, S. Cavalli, and D. De Fazio *J. Chem. Phys.* **109**, 3792 (1998)

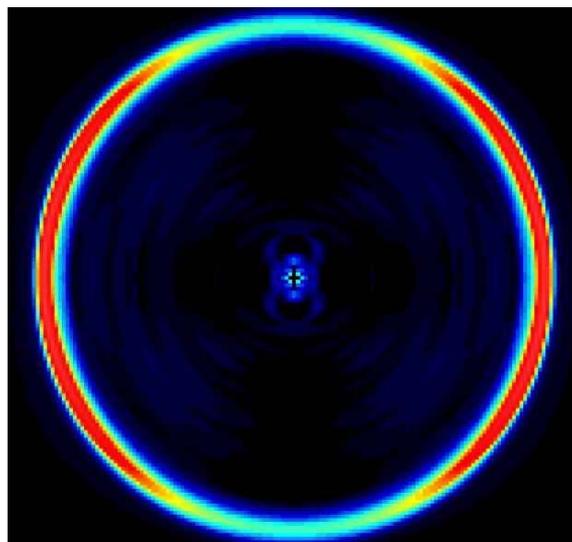
Molecular videos: watching chemical change with ultrashort lasers

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In this contribution we will show recent experimental work where fast molecular processes have been investigated directly through the combination of ultrashort laser pump-probe schemes with the velocity map imaging technique. Different versions of the technique will be presented: selective detection of fragments in given quantum states, nonselective fragment detection and Coulomb explosion detection with intense infrared pulses. The application of these techniques has allowed us to explore ultrafast dynamics on excited state surfaces in molecules and clusters¹⁻⁴. Examples will be presented on $(\text{CH}_3\text{I})_2$ dissociation and on the predissociation process in the *B*-band of CH_3I .



¹ J. Durá, R. de Nalda, G.A. Amaral, L. Bañares, *J. Chem. Phys.* **131**, 134311 (2009)

² R. de Nalda, J. Durá, A. García-Vela, J.G. Izquierdo, J. González-Vázquez, L. Bañares, *J. Chem. Phys.* **128**, 244309 (2008)

³ J. Durá, R. de Nalda, J. Álvarez, J. G. Izquierdo, G.A. Amaral, L. Bañares, *Chem Phys Chem* **9**, 1245 (2008)

⁴ R. de Nalda, J.G. Izquierdo, J. Durá, L. Bañares, *J. Chem. Phys.* **126**, 021101 (2007)

Interferences between resonances localized in metal nanostructures supported on metal surfaces

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Recently, manipulation of adsorbed atoms and molecules with atomic precision as offered by Scanning Tunnelling Microscopy (STM) allowed the creation of metal atom chains aligned on a metal surface (see e.g.¹⁻²). Unoccupied electronic states localized on the chain have been evidenced and shown to correspond to a one-dimensional (1D) free-electron like band quantized on the finite size object¹⁻². It corresponds to an electron propagating along the structure and develops from the hybridization of excited electronic states of sp symmetry localized on the individual adatoms²⁻³.

In this communication we present a theoretical study of the 1D sp-band of excited electronic states localized on Cu monoatomic chains supported on a Cu(111) surface⁴. A wave packet propagation approach is employed for the description of the electron dynamics and *ab initio* density functional calculations were carried out to obtain the corresponding one-electron potentials^{3,5-6}. The 1D sp-band appears as a quasi-stationary state, i.e. as a scattering resonance in the electronic continuum of the metal substrate. Energies and lifetimes of the chain-localized electronic states have been computed and compared with experimental measurements^{2,4}. We show that an excited electron can propagate ~1 nm along the chain before it escapes.

The lifetime of the resonance can be dramatically increased in the case of a double chain. Indeed, a parallel double chain of Cu metal atoms adsorbed on a Cu(111) metal surface can guide an excited electron for distances exceeding 10 nm and, thus, act as a nanowire insulated from the substrate⁷. This system has no macroscopic analog since conventional insulation of the wire from the surrounding is absent. Instead, the insulating effect is brought by a quantum mechanical phenomenon first addressed by von Neumann and Wigner, and known as formation of bound states in the continuum. The above result should be of general occurrence in atomic and molecular physics and can be explained within the framework of the theory of interacting resonances: the two quasi-stationary states localized on the Cu chains appear as two interacting resonances in the substrate continua leading, for the proper distance between the two chains, to the formation of a very long-lived and a very short-lived resonance.

¹ N. Nilius *et al.*, *Science* **297**, 1853 (2002)

² S. Fölsch *et al.*, *Phys. Rev. Lett.* **92**, 056803 (2004)

³ F.E. Olsson *et al.*, *Phys. Rev. Lett.* **93**, 206803 (2004)

⁴ S. Díaz-Tendero *et al.*, *NanoLetters* **8**, 2712 (2008)

⁵ A.G. Borisov *et al.*, *Phys. Rev. B* **59**, 10935 (1999)

⁶ S. Díaz-Tendero *et al.*, *Phys. Rev. B* **77**, 205403 (2008)

⁷ S. Díaz-Tendero *et al.*, *Phys. Rev. Lett.* **102**, 166807 (2009)

Bohmian mechanics: A novel tool to explore the physics and chemistry of atoms and molecules

A. S. Sanz^(a),

A fast path integral method for polarizable force fields. Application to liquid water and Ice

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Computer simulations based on classical statistical mechanics offer a powerful tool for the study of complex chemical systems. However, for systems involving hydrogen atoms at low to moderate temperatures quantum mechanical (zero point energy and tunneling) effects become important and the predictions of classical mechanics become unreliable. In such cases the inclusion of quantum mechanical fluctuations in the nuclear degrees of freedom is essential for an accurate description. One appealing but computationally demanding approach to this problem is provided by the imaginary time path integral expression for the quantum mechanical partition function. A quantum simulation of an imaginary time path integral typically requires around n times more computational effort than the corresponding classical simulation, where n is the number of ring polymer beads or imaginary time slices used in the calculation. Here we present a new technique in order to improve the previous estimate. It is based on the decomposition of the potential function into a sum of slowly and rapidly varying contributions. As the slowly varying contribution changes only slightly over the length scale of the ring polymer, it can be evaluated on a contracted ring polymer with fewer than the full n beads, significantly reducing in this way the required computational cost. The method can be applied in simulations where different types of pairwise additive and polarizable empirical force fields [1,2] are employed for the description of the intermolecular interactions. Here we develop and test this idea for systems with many body polarizable force fields [2]. The method is illustrated with simulations of liquid water at 300 K and hexagonal ice at 100 K using a recently developed flexible and polarizable Thole-type potential energy model, TTM3-F [3]. It is shown that with the appropriate choice of the parameters the method provides accurate results with little more than classical computational effort in the limit of large system size.

[1] T. E. Markland and D. E. Manolopoulos, *Chem. Phys. Lett.* **464**, 256 (2008)

[2] G. S. Fanourgakis, T. E. Markland, and D. E. Manolopoulos, *J. Chem. Phys.* **131**, 094102 (2009)

[3] G. S. Fanourgakis and S. S. Xantheas, *J. Chem. Phys.* **128**, 074506 (2008)

Excited state nonadiabatic molecular dynamics: energy funneling in light harvesting dendrimers

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Dendrimer macromolecules can be thought of as arrays of coupled chromophores with the energy of each unit depending on the backbone structure and conformation. There is a deep interplay between the strength of the coupling between units, dephasing and vibrational energy dissipation channels, and the nature of the energy transfer. Absorption of light in organic solar cells creates excitons that diffuse to a heterojunction, where charge separation occurs. For an efficient photon-to-current conversion, exciton transport process must occur in a time scale shorter than deactivation. It is then critical that we understand the mechanisms for exciton transport and explore the chemical and physical properties that can help speed the process.

Excited state nonadiabatic molecular dynamics simulations are used to study the nature of the energy transfer in dendrimers building blocks, between two-, three- and four-ring linear poly-phenylene ethynylene (PPE) units linked by meta-substitutions. Dendrimers built from these building blocks have been experimentally shown to undergo, upon excitation, highly efficient and ultrafast unidirectional energy transfer. The simulations start by an initial vertical excitation to the S_4 that is localized on the two-ring unit. We observe ultrafast and mostly one-directional $S_4 \rightarrow S_3 \rightarrow S_2 \rightarrow S_1$ electronic energy transfer, concomitant with an also ultrafast two-ring \rightarrow three-ring \rightarrow four-ring vibrational energy transfer. The $S_{n+1}-S_n$ ($n=3-1$) energy gaps and nonadiabatic couplings are strongly influenced by the different nuclear motions in the different potential energy surfaces. Subsequent to a significant $S_{n+1} \rightarrow S_n$ electronic population transfer, a rapid increase of the $S_{n+1}-S_n$ energy gaps and decrease of the corresponding values for S_n-S_{n-1} gaps are observed. In consequence, the S_{n+1} and S_n states become less coupled while the S_n while S_{n-1} become more coupled. This behavior guarantees the successful $S_{n+1} \rightarrow S_n \rightarrow S_{n-1}$ unidirectional energy transfer associated to the efficient energy funneling in light-harvesting dendrimers.

“Nonadiabatic molecular dynamics simulations of the energy transfer between building blocks in a phenylene ethynylene dendrimer” S. Fernandez-Alberti, Valeria D. Kleiman, S. Tretiak, and Adrian E. Roitberg, J. Phys. Chem A, 113, 7535-7542, (2009).

Unidirectional energy transfer in conjugated molecules: the crucial role of high frequency C(triple)C bonds” S. Fernandez-Alberti, Valeria D. Kleiman, S. Tretiak, and Adrian E. Roitberg, submitted to J. Phys. Chem. Lett. (2010).

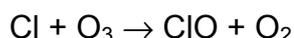
Ab initio potential energy surface and quasiclassical trajectory studies of the Cl + O₃ reaction

Jesús F. Castillo^a, Bruno Martínez-Haya^b, Francisco J. Aoiz^a and Luís Bañares^a

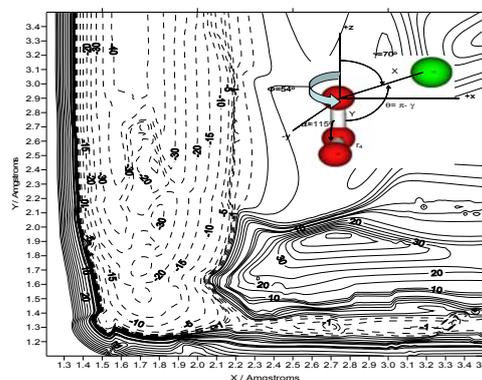
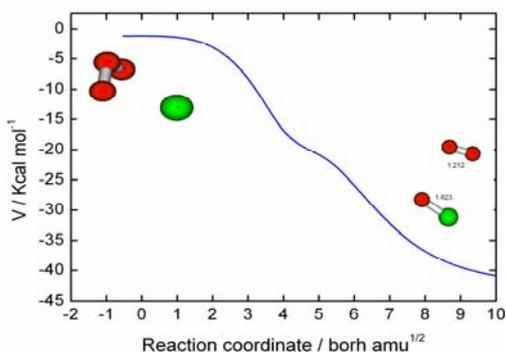
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We present the results *Ab initio* and Quasiclassical Trajectory (QCT) calculations for the reaction



which is an elementary step in a catalytic cycle that leads to the destruction of ozone in the stratosphere. The calculations are carried out employing a global full dimensional potential energy surface (PES) constructed by interpolation of *Ab Initio* Quantum Chemistry data using the modified Sephard interpolation method developed by Collins and co-workers [1]. *Ab Initio* data points (energy, gradients and hessian matrix elements) have been calculated at the Quadratic Configuration Interaction with Single and Double excitations, QCISD/aug-cc-pVDZ level of theory. This is the first global fully *Ab Initio* PES ever constructed for the Cl + O₃ reaction. QCT calculations for ground state and vibrationally excited states of O₃ have been carried out for several collision energies. Detailed comparisons of calculated product vibrational distributions, integral and differential cross sections with experimental determinations [2-4] will be presented and discussed.



Reaction path and contour plot of the *ab initio* PES

¹ Collins M. A.. *Theor. Chem. Acc.* **2002**, *108*, 313

² Zhang J., Lee Y. T. *J. Phys. Chem. A.* **1997**, *101*, 6485.

³ Matsumi Y., Nomura S., Kawasaki M., Imamura T. *J. Phys. Chem.* **1996**, *100*, 176.

⁴ Baumgärtel S, Delmdahl R. F., Gericke K.-H, Tribukait A., *Eur. Phys. J. D.* **1998**, *4*, 199

Quantum mechanical description of vibrations in molecules and solids

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Time permitting, I shall present an overview of our recent work on the quantum mechanical description of anharmonic vibrations in molecules and in solids.

An exact and general approach to study molecular vibrations is provided by the Watson Hamiltonian. Within this framework, it is customary to omit the contribution of the terms with the vibrational angular momentum and the Watson term, especially for the study of large systems. We discovered that this omission leads to results which depend on the choice of the reference structure and proposed that the self-consistent solution leads to the optimum choice of molecular reference structure¹. The self-consistent reference geometry (or structure) does not correspond to stationary point of the potential energy surface and as a result we had to develop a way to determine rectilinear vibrational coordinates which satisfy the Eckart's conditions at non-stationary points of the PES². Finally, the applicability of the Watson Hamiltonian for the description of non-linear molecules (near linearity) has always been questioned, since the Jacobian of the transformation, that leads to the Watson Hamiltonian, vanishes at the linear configuration. This results in singular behaviour of the Watson Hamiltonian, giving rise to serious numerical problems in the computation of vibrational spectra. In Ref. 3, we analysed the problem and proposed a simple solution.

In solids⁴, we studied the structural effects produced by the quantization of vibrational degrees of freedom in periodic crystals at zero temperature. To this end we introduced a methodology based on mapping a suitable subspace of the vibrational manifold and solving the Schrödinger equation in it. A number of increasingly accurate approximations ranging from the quasiharmonic approximation QHA to the vibrational self-consistent field VSCF method and the exact solution were studied. These methods were initially applied to study a linear H-F chain and very recently in an attempt to give an ab initio explanation of the Ubbelohde effect⁵.

¹ I. Scivetti, J. Kohanoff, N. Gidopoulos, *Phys. Rev. A* **80**, 022516 (2009)

² I. Scivetti, J. Kohanoff, N. Gidopoulos, *Phys. Rev. A* **79**, 032516 (2009)

³ I. Scivetti, J. Kohanoff, N. Gidopoulos, *Int. J. Quant. Chem.* in press (2010)

⁴ I. Scivetti, N. Gidopoulos, J. Kohanoff, *Phys. Rev. B* **78**, 224108 (2008)

⁵ JM Robertson, AR Ubbelohde, *Proc. R. Soc. A* **170**, 222 (1939)

Genetic algorithms search methods and applications in molecular clusters

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The structures and stability of molecular clusters play a key role for describing physical and chemical properties. The determination of the minima on the potential energy surface is considered crucial for at least semiquantitative analysis, thus many theoretical studies have been devoted to the goal of global optimization. However, as the number of local minima rises quasiexponentially with cluster size, global geometry optimization becomes very difficult for larger clusters, and particularly for weakly bound vdW ones. Recently, interest has been shown in the use of the genetic algorithm (GA) to solve the problem of global optimization¹. Genetic algorithms are efficient heuristic search methods based on Darwinian evolution with powerful characteristics of robustness and flexibility to capture global solutions of complex optimizations. The GA approach is a powerful tool and it can be used not only as a replacement of traditional optimizations, but may extend and improve them – in general, better performances are reached, by using hybrid methods.

A simple GA uses repeated trials of the Selection-Crossover-Mutation sequence from an initial population (IP) as can be seen in Figure 1.

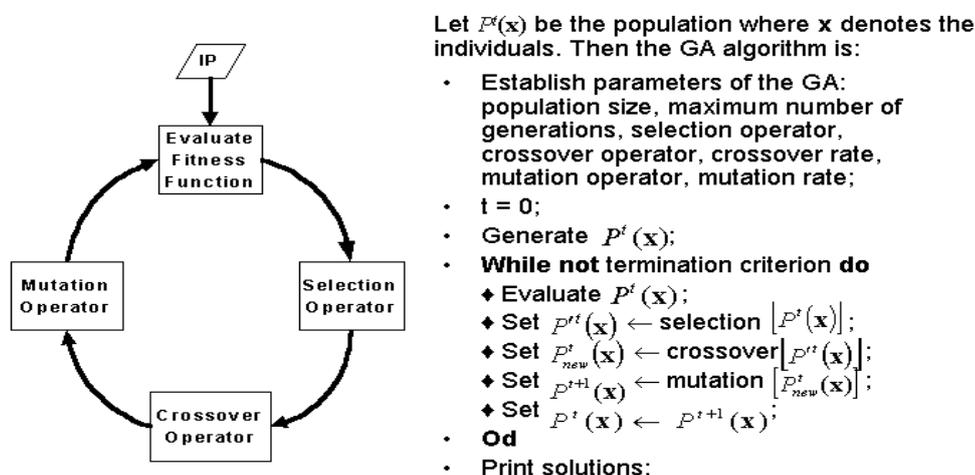


Figure 1. Scheme of a simple Genetic Algorithm.

In this study, we will use a GA² to explore an *ab initio*-based surface of He_n-ICl clusters³. Various local minimum structures are located and their stability is analysed. The actual results are compared with previous ones and the efficiency of the present method is discussed.

¹ R. Judson, *Rev. Comp. Chem.* **10**, 1 (1997)

² G. Winter, *et al*, *Soft Comp.* **9**, 299 (2005)

³ A. Valdés, *et al.*, *J. Chem. Phys.* **125**, 014313 (2006)

Strong field effects in halomethanes

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Control of nuclear and electron dynamics in molecules is a hot topic in chemistry and molecular physics. In view of the easy cleavage of halogen atoms upon irradiation, halomethanes (CH_2XY) are good candidates for laser-driven selective bond dissociation. In the presence of strong fields, multiphoton and tunnel ionization can additionally ionize the system and create electronic wavepackets. In this contribution we present the effect of strong fields on several halomethanes, e.g. CH_2BrI and CH_2I_2 . In CH_2BrI momentum-dependent photodissociation is experimentally observed when using ultrashort IR pump pulses with peak intensities of 10^{14} W/cm².¹ Using a dressed-state picture based on accurate multiconfigurational CASSCF potential energy surfaces including spin-orbit coupling it can be seen that while dissociation for left- and right-going wave packets is roughly symmetric for weak coupling between the potentials, bond breaking is asymmetric for strong coupling.² In CH_2I_2 strong IR pump pulses in the regime of tunnel ionization create vibrational wavepackets on several electronic states of the ion which can be changed with the chirp of the pulse. Our dynamical simulations on coupled CASSCF potentials illustrate the composition of the created electronic wavepacket.³

¹ S. R. Nichols, T. Rozgonyi, B.J. Pearson, T. Weinacht, *Phys. Rev. A* **79** 043407 (2009).

² J. González-Vázquez, L. González, S. R. Nichols, T. Weinacht, T. Rozgonyi, *submitted* (2010).

³ D. Geißler, T. Rozgonyi, J. González-Vázquez, L. González, S. R. Nichols, T. Rozgonyi, *submitted* (2010).

The stability of a crystal with diamond structure for patchy particles with tetrahedral symmetry

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The study of the behaviour of anisotropic particles has attracted significant attention in recent years. Initially the interest arose because they were seen as simplified models of proteins and, even though these models are extremely simple, they have been found to reproduce some characteristics of the phase behaviour of proteins.¹⁻³ More recently a number of experimental groups have developed new methods to produce nanoparticles and colloids with anisotropic shapes or interactions and this has also motivated many theoretical and simulation studies.^{4,5} One target in this field is to produce particles with tetrahedral symmetry that assemble in a diamond crystal, which is motivated by its possible applications in photonics.⁶ As a first step to understand the factors that could lead to the appearance of low density solids and to study the mechanism for the nucleation we have studied the phase diagram of anisotropic particles with tetrahedral symmetry by computer simulation. We found that the diamond crystal is competitive with a body centred cubic crystal and that the diamond crystal is stabilized with respect to the body centred cubic crystal as the range of the potential decreases. We have also performed preliminary simulations of the interface between a fluid and the body centred cubic crystal and between the fluid and the diamond crystal. Our results show that, at sufficiently low pressures, it is quite likely that both solids grow into a diamond crystal with some defects.⁷

¹ N. Kern and D. Frenkel, *J. Chem. Phys.* **118**, 9882 (2003).

² H. Liu, S.K. Kumar, F. Sciortino, and G.T. Evans, *J. Chem. Phys.* **130**, 044902 (2009).

³ E.G. Noya, C. Vega, J.P.K. Doye and A.A. Louis, *J. Chem. Phys.* **127**, 054501 (2007).

⁴ S.C. Glotzer and M.J. Solomon, *Nat. Mater.* **6**, 557 (2005).

⁵ J.P.K Doye, A.A. Louis, I.-C. Lin, L.R. Allen, E. G. Noya, A.W. Wilber, H.C. Kok, and R. Lyus, *Phys. Chem. Chem. Phys.* **9**, 2197 (2007).

⁶ A.-P. Hynninen, J.H.J. Thijssen, E.C.M. Vermolen, M. Dijkstra, and A. Van Blaaderen, *Nat. Mat.* **6**, 202 (2007),

⁷ E.G. Noya, C. Vega, J.P.K. Doye and A.A. Louis, submitted.

Understanding of relation between chemical force and current at atomic scale

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Fast development of real space local probe techniques such as Scanning Probe Microscope (SPM) has allowed the precise control and the modification of surfaces at the atomic scale. While standard STM image procedures operate mostly at so called the tunneling regime, more and more applications take place in the near-to-the contact regime¹ during last years. In this regime, the probe proximity strongly modifies the surface structure making the precise interpretation of experimental results more complicated.

From an elementary quantum mechanics course we learned that the tunneling current grows exponentially with the decrease of the length of the tunneling barrier or, in context of STM measurements, to the tip-sample distance. However, this basic assumption has to be carefully re-examined at distance where the onset of short-range chemical interaction between the probe apex and the surface adatoms takes place^{2,3}.

In this work, we will discuss key effects playing an important role during the formation of the atomic contact between tip and sample and the electron transport through the contact. Here, we combine STM/AFM measurements, first principle DFT total energy methods and calculations of the electron currents based on Green's function techniques². First, we will discuss the mechanism of the resonant tunneling through 'dangling bond' states of Si adatoms on the Si(111)-(7x7) surface⁴. In the near-to-contact regime, the substantial decrease of the current, almost to zero, is both experimentally and theoretically observed. We will also present recent results on metal surfaces⁵.

¹ F.J. Giessibl *Mod. Phys.* **75** 949 (2003).

² J.M. Blanco *et al Phys. Rev. B* **70** 085405 (2004) .

³ Y. Sugimoto *et al Nature* **446**, 64 (2007) .

⁴ P. Jelínek *et al Phys. Rev. Lett.* **101** 176101 (2008).

⁵ M. Ternes *et al* (in preparation).

On the Bonding Interpretation of H₂SO₄, HNO₃, HClO₄, and O₃.

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The bonding nature of the non-hydroxyl oxygen atoms of the familiar acids sulphuric [(OH)₂SO₂], nitric (HONO₂), and perchloric (HOClO₃) is explained without using such *ad hoc* concepts of circular logic like “hypervalency”.¹ It is proposed here for the first time and confirmed through the help of coupled-cluster RCCSD(T) calculations, that the S(-O)₂, N(-O)₂, and Cl(-O)₃ bonding occurs by transfer of the electron pair densities of the central atoms, S, N, and Cl to the first excited state, ¹D, of the non-hydroxyl O atoms.

In the case of the X-state of O₃, a careful analysis of the MRCI wavefunction does not support the biradical character, adopted long ago by the scientific community.² It can be viewed as a excited O(¹D) atom that binds to the excited O₂(*a*¹Δ_g) molecular state.

¹ A. Kalemos and A. Mavridis *J. Phys. Chem. A* **113**, 13972 (2009).

² A. Kalemos and A. Mavridis *J. Chem. Phys.* **129**, 054312 (2008).

Rationalizing the S(¹D) + H₂ cold reaction dynamics using a simple semi-classical statistical model

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In the last few years, quantum and semi-classical statistical models have proven fairly accurate at predicting reactive cross-sections as well as state/spatial distributions in the products of triatomic insertion processes such as the title reaction. The main advantages of such theoretical treatments are numerical simplicity and interpretative power.

A simple semi-classical statistical model is presented here and its relevancy down to very low collision energies (5-120K) is evidenced for the S(¹D)+ H₂ reaction by comparison with recent exact quantum scattering calculations (*M. Lara et al.*) and molecular beams experiments (*M. Costes et al.*)

Approximating electronic correlations with Reduced Density Matrix Functional Theory (RDMFT)

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In RDMFT, the one-body reduced density matrix (1-RDM) is the fundamental density i.e. it plays the same role as the electronic density in DFT. The obvious advantage is that the kinetic energy is a simple explicit functional of the 1-RDM. Consequently, no kinetic energy contributions exist in the exchange and correlation term. In RDMFT approximate expressions of the total energy are written in terms of the 1-RDM and minimized with respect to 1-RDM under the N-representability conditions which guarantee that the optimal 1-RDM corresponds to a many-body wave function.

RDMFT is only relatively recently exploited for realistic calculations in molecules and solids. We review the basic ideas of RDMFT, the most important functionals and promising applications to prototype finite and periodic systems. These applications include calculations of dissociation energy plots, atomization energies, ionization potentials, the fundamental gap of semiconductors and insulators, as well as the calculation of the correlation energy of the homogeneous electron gas.

The aim of developing RDMFT is not to replace well established and widely used theories but to develop an efficient method that could give answers to problems that the results of established methods deviate from experiment.

Theoretical Study of the Predissociation of the A²Π States of ZnF Incorporating Quasi-Diabatisation of the Spin-Orbit Coupling

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Zinc fluoride, ZnF, is a ionic molecule belonging to the family of the monofluorides and monoxides of 3d metals, which has been recently investigated by spectroscopic methods to elucidate the characteristics of their chemical bonds. Even though ZnF can be easily produced by the exothermic reaction ($\Delta E = 1.55$ eV) of zinc vapor with F₂ gas, this system had rarely been investigated. Of particular interest for the vibrational spectroscopy of Zn compounds is the abundance of the various stable isotopes of this element: their natural abundances are ⁶⁴Zn (48.6 %), ⁶⁶Zn (27.9 %), ⁶⁸Zn (18.8 %), ⁶⁷Zn (4.1 %), and ⁷⁰Zn (0.6 %) giving a specific signature in the spectra.

The electronic states of ZnF diatomic have already been studied¹. The lowest ²Π states exhibit an avoided crossing in the Franck-Condon Region of the X²Σ⁺. The only experimental study of the rovibronic transition X → A gives results that can not be understood without considering non-adiabatic interactions between both A²Π states².

The quasi-diabatisation of the A²Π states and of the spin-orbit coupling terms has been achieved, giving one very well bound component, responsible for the long life-time states observed by spectroscopists. The second Π component is repulsive, leading to pre-dissociative states.

The lowest two ²Π and lowest two ²Σ⁺ states potentials are based on highly correlated *ab initio* calculations using the MRCI method, pseudo-potentials and aug-cc-pVQZ-PP basis sets for both Zn and F atoms. The spin-orbit coupling terms between all these states are considered.

¹ S. Hayashi, C. Léonard and G. Chambaud *J. Chem. Phys.* **129**, 044313 (2008)

² G. D. Rochester and E. Olsson *Z. Physik*, **114**, 495 (1939)

Oriented collision dynamics of simple chiral molecules

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The phenomenon of chirality (handedness) occurs for molecular systems that can exist in two forms differing by being mirror images of each other. It has numerous and interesting implications in chemistry and biochemistry, especially concerning the role of specific enantiomers in reactions proceeding enantioselectively, when chiral reactants or catalysts are involved, or in presence of an external chiral field. Amazingly, terrestrial life involves only the L enantiomers of amino acids, and the D enantiomers of sugars, a fact known as the homochirality of life. The puzzling problems related to the origin of homochirality in nature have encouraged long-standing efforts to clarify its origin [1] and a long lasting search for mechanisms responsible for the generation of enantiomeric excess.

A reliable hypothesis for these mechanisms, but still not sufficiently investigated, attributes chirality discrimination to molecular collisions, and has been discussed in Ref. [3] where it has been examined also the possibility that collisions take place in environments characterized by rotary or whirling motions. This hypothesis can be verified combining experimental and theoretical efforts.

In this view, extensive classical dynamics simulations of oriented collisions of rare gas atoms with prototypical chiral molecules, such as hydrogen peroxide and hydrogen persulfide are presented. Models for the intermolecular and intramolecular interactions are based on previous quantum chemical calculations [4,5]. The phenomenon of right-left asymmetry in scattering directions is documented both by exemplary single trajectories and by angular distributions obtained by statistical averagings [6].

[1] Cline, D. B. *European Review* Cambridge University Press 2005, 13, 49.

[2] Rikken, G. L. J. A.; Raupach, E. *Nature* 2000, **405**, 932.

[3] Aquilanti, V.; Maciel G. S. *Orig. Life Evol. Biosph.* 2006, **36**, 435.

[4] Maciel G. S.; Barreto P. R. P.; Palazzetti F.; Lombardi A.; Aquilanti V. *J. Chem. Phys.* 2008, **129**, 164302.

[5] Barreto P. R. P.; Vilela A. F. A.; Lombardi A.; Maciel G. S.; Palazzetti F.; Aquilanti V. *J. Phys. Chem. A* 2006, **111**, 12754.

[6] Lombardi, A.; Palazzetti, F.; Maciel, G.; Aquilanti, V.; Sevryuk, M. B. *Int. J. Quant. Chem.* 2010, in press.

Trends in Metal Oxide Stability for Nanorods, Nanotubes and Surfaces

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The search for cleaner and more sustainable forms of energy provides a strong impetus to the development of more affordable, active, selective and stable new catalysts to convert solar radiation into fuels. For such a task, one important property of oxides is their high stability in harsh oxidizing environments compared to their pure metal counterparts^{1,2}. The structure of oxide nanoparticles may be determined by the surface energy¹. Typically, oxide catalysts are in the form of nanoparticles or highly porous materials. The catalytic properties of these materials are determined to a high degree by the surface, and control of the surface structure will allow control of the reactivity. However, formation energies of metal oxide surfaces are difficult to measure experimentally, and only a few values are available in the literature. This makes the calculation of trends in surface and nanostructure energies an essential first step in understanding the properties of oxide catalysts, and the eventual design of novel catalytic materials.

For the case of 15 different rutile and 8 different perovskite metal oxides, we find that the density functional theory (DFT) calculated formation energies of (2,2) nanorods, (3,3) nanotubes, and the (110) and (100) surfaces may be described semi-quantitatively by the fraction of metal–oxygen bonds broken and the bonding band centers in the bulk metal oxide¹.

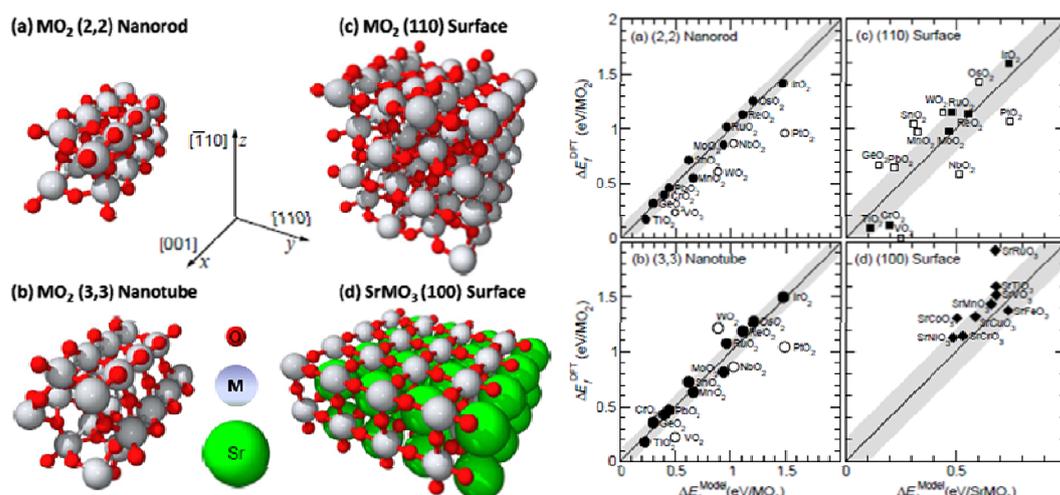


Fig. 1: Structural schematics for several MO₂ and SrMO₃ nanostructured systems (M=Ti, V, Cr, Mn, Os, Re, W, etc...); and DFT calculated formation energy E_f^{DFT} vs. model prediction E_f^{Model}

¹ J. I. Martínez *et al.*, accepted in *Phys. Rev. Lett.* (2010)

² J. I. Martínez *et al.*, accepted in *Angew. Chem. Int. Ed.* (2010)

Chemical dynamics simulations of Ar, CO₂ and NO scattering from a perfluorinated self-assembled monolayer surface

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Chemical dynamics simulations were performed to study energy transfer in collisions of X (with X=Ar, CO₂ and NO) with a perfluorinated octanethiol self-assembled monolayer (F-SAM) surface. All-atom (AA) and united-atom (UA) models¹ were used for the F-SAM surface along with accurate X + F-SAM potentials, developed from high-level *ab initio* calculations.

The simulations provide different energy transfer efficiencies for CO₂+F-SAM² and Ar+F-SAM³ when AA and UA models are employed. The translational $P(E_t)$ and ro-vibrational $P(v,J)$ distributions of the scattered species obtained with the AA model^{2,3,4} are in excellent agreement with the experimental results, and the results obtained with the UA model being is worst agreement with experiment. However, recently an improved UA model was developed that compares very well with the AA model results for the CO₂ $P(v,J)$ distributions.^{1,5}

Our simulations show that most of the $P(E_t)$ and $P(v,J)$ distributions are consistent with two mechanisms of energy transfer: an impulsive mechanism, and a much longer duration mechanism where accommodation of the rotational and translational degrees of freedom takes place. Accommodation of the bend vibrational mode of CO₂ takes more time and does not take place in the time scale of the collision process.^{5,6}

Scattering of NO from F-SAM was also studied⁷ and the results will also be presented at the conference.

¹J. J. Nogueira, E. Martinez-Nunez, S. A. Vazquez *J. Phys. Chem. C* **113**, 3300 (2009)

²J. J. Nogueira, S. A. Vazquez, O. Mazyar, W. L. Hase, B.G. Perkins, D. J. Nesbitt, E. Martinez-Nunez *J. Phys. Chem. A* **113**, 3850 (2009)

³S. A. Vazquez, J. R. Morris, A. Rahaman, O. A. Mazyar, G. Vayner, S. V. Addepalli, W. L. Hase and E. Martinez-Nunez *J. Phys. Chem. A* **111**, 12785 (2007)

⁴E. Martinez-Nunez, A. Rahaman, W. L. Hase *J. Phys. Chem. C* **111**, 354 (2007)

⁵J. J. Nogueira, S. A. Vazquez, U. Lourderaj, W. L. Hase, E. Martinez-Nunez *J. Phys. Chem. C* (submitted)

⁶U. Lourderaj, E. Martinez-Nunez, W. L. Hase *J. Phys. Chem. A* **111**, 10292 (2007)

⁷Z. Homayoon, J. J. Nogueira, S. A. Vazquez, E. Martinez-Nunez, (in preparation)

Stimulated Raman Spectroscopy for the Study of Collisional Energy Transfer: Determination of Rotational State-to-State Relaxation Rates in Acetylene.

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An experimental technique for the direct measurement of rotational state-to-state collisional relaxation rates in gas phase molecules is presented. The scheme is based on the sequential use of two stimulated Raman processes in a pump-probe configuration, as depicted in Figure 1. The first process, employing two pulsed laser beams, pumps population from the $v=0$ ground vibrational state to the $v=1$ excited state of the molecule. The linewidth of the two lasers is narrow enough to populate a single rotational level J_p in $v=1$. After an adjustable delay, the second Raman process, in this case a quasi continuous (q-cw) stimulated Raman loss setup, is used to probe the population in the different rotational levels in $v=1$, including the initially populated J_p . By changing the delay while keeping the frequencies of the pump and probe experiments fixed the evolution of the population in any rotational level can be closely monitored. This procedure is carried out repeatedly to obtain evolution data for all the rotational levels in $v=1$ that are significantly populated. Figure 2 shows as an example the set of population evolution data obtained for acetylene at 155 K and 1 mbar when population is initially pumped to the $v_2=1, J=9$ level.

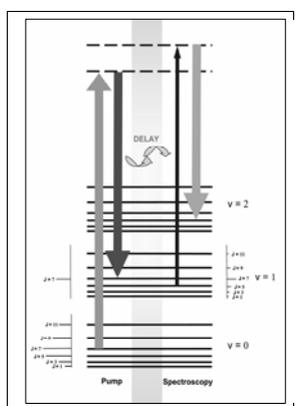


Figure 1: The pump-probe scheme.

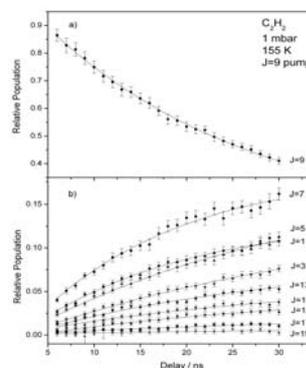


Figure 2: Evolution of rotational populations in $v_2=1$.

Several sets of data like the one in Figure 2 are collected by pumping population to different rotational levels. The data are then used to find a solution, through an iterative algorithm, to the master equation $dn(t) = \mathbf{k}n(t)Pdt$ that describes the evolution of the rotational populations \mathbf{n} as a function of the number of collisions (pressure \times time) and the rate constant matrix \mathbf{k} . The final result of this calculation is the \mathbf{k} matrix that produces the best overall fit of the calculated evolution of the populations to the experimental data. The continuous lines in figure 2 represent this evolution as described by the \mathbf{k} matrix obtained from the fit. A detailed experimental description of the technique as well as the results of its first application to the molecule of acetylene will be presented. The rate constants thus obtained will be compared to those generated by the most commonly used fitting and scaling laws when they are applied to the same set of experimental data.

A study of CH₄/H₂O ices by infrared spectroscopy

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The coexistence of solid methane and water ice has been observed in outer Solar System objects, and in interstellar ice mantles^{1,2}. It has been also conjectured that interactions between methane and water ice might be of relevance for the climate of Solar System objects like Titan³. To extract valuable information from the observed spectra (temperature, pressure, chemical speciation, etc.) thorough laboratory studies are required. This work presents an investigation on ice mixtures of methane and water, studied by infrared spectroscopy. The spectra provide evidence of a distorted CH₄ structure, characterized by an absorption band at 2900 cm⁻¹, forbidden by symmetry in the pure solid. We present an estimation of the amount of distorted CH₄ trapped in the water ice structure and its dependence on the ice generation procedure. In addition, the presence of methane clusters inside the sample directly affects the frequency and intensity of the dangling bonds of water. When CH₄ is deposited on water ices, the adsorption process follows a Type I isotherm graphic, indicating the microporous nature of the ices. We have also determined the CH₄:H₂O desorption energy and measured the dependence of the position and widths of the IR bands as a function of the stoichiometry of the samples^{4,5}.

¹E. L. Schaller and Brown, *Astrophys. J.* **670**, L49-L51 (2007).

²K. I. Öberg, et al., *Astrophys. J.* **678**, 1032-1041, (2008).

³L. F. Voss, et al., *J. Geophys. Res.*, **112**, E05002 (2007).

⁴O. Gálvez, B. Maté, V.J. Herrero, and R. Escribano, *Astrophys. J.* **703**, 2101 (2009).

⁵V.J. Herrero, O.Gálvez, B. Maté, and R. Escribano, *Phys. Chem. Chem. Phys.* **12**, 3164 (2010).

Electric and elastic properties of wurtzite nanowires

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Nanowires and in general nanostructures present surface energy that makes their properties size-dependent. Using first principles (Hartree-Fock and Density Functional Theory) methods, we have calculated piezo-electric and elastic properties of wurtzite [0001] nanowires, in particular *ZnO* and *AlN* nanowires. For *ZnO*, we have studied the effect of partial substitution of zinc by mercury and found that this leads to the significant enhancement of piezo-electric properties. For aluminum nitride, we have further built a classical, Finite Element (FEM), model of a nanowire, using the bulk and surface energy model with parameters derived from *ab initio* calculations. The elastic properties obtained with the FEM model compare very well with those obtained with the full *ab initio* calculations. The FEM continuum model can be used to model similar nanostructures in ranges of sizes or geometries where *ab initio* calculations are not feasible, and also to predict the bending or twisting properties of nanowires where *ab initio* methods are not yet available.

"Piezoelectric Properties of *AlN*, *ZnO*, and *Hg_xZn_{1-x}O* Nanowires by First-Principles Calculations" A Mitrushchenkov, R Lingerri, and G Chambaud, *J.Phys.Chem.* **113** 6883-6886(2009)

"Towards an elastic model of wurtzite *AlN* nanowires" A Mitrushchenkov, G Chambaud, J Yvonnet, and Q-C He, *Nanotechnology*, in press(2010)

"Finite element model of ionic nanowires with size-dependent mechanical properties characterized by *ab initio* calculations" J. Yvonnet , A. Mitrushchenkov, G. Chambaud, Q.-C. He, submitted to CMAME

Ab initio studies of propene epoxidation at noble metal nanocatalysts

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Nanometer-sized gold particles have been reported as promising catalysts for the direct propene epoxidation reaction¹. Motivated by these results, recent experiments by S. Vajda and collaborators^{2,3} have studied the activity for this reaction of alumina-supported gold and silver nanocatalysts. In the case of gold, a remarkable activity and selectivity towards propene oxide formation is found for small sub-nm clusters (Au₇-Au₁₀). Silver nanoparticles (9-23 nm diameter) are also found active for propene oxide production, with the selectivity being strongly dependent on particle size and reaction temperature. In parallel to the experiments, ab-initio DFT simulations were performed to study both the stability of key reaction intermediates and the energy barriers for either acrolein or propene oxide formation. In the case of gold, the simulations confirm the superior catalytic activity of the small sub-nm clusters, and also a key role of the alumina surface oxygen anions during the formation of reaction intermediates. In the case of silver nanoparticles, the size- and corresponding morphology dependent theoretical activity and selectivity are in good accord with experimental observations: the edge sites that are more abundant in smaller particles enhance selectivity towards acrolein, whereas nanoparticle facet sites, which dominate for larger particles, preferentially form propene oxide.

¹ T. Hayashi, K. Tanaka and M. Haruta, *J. Catal.* **178**, 566 (1998)

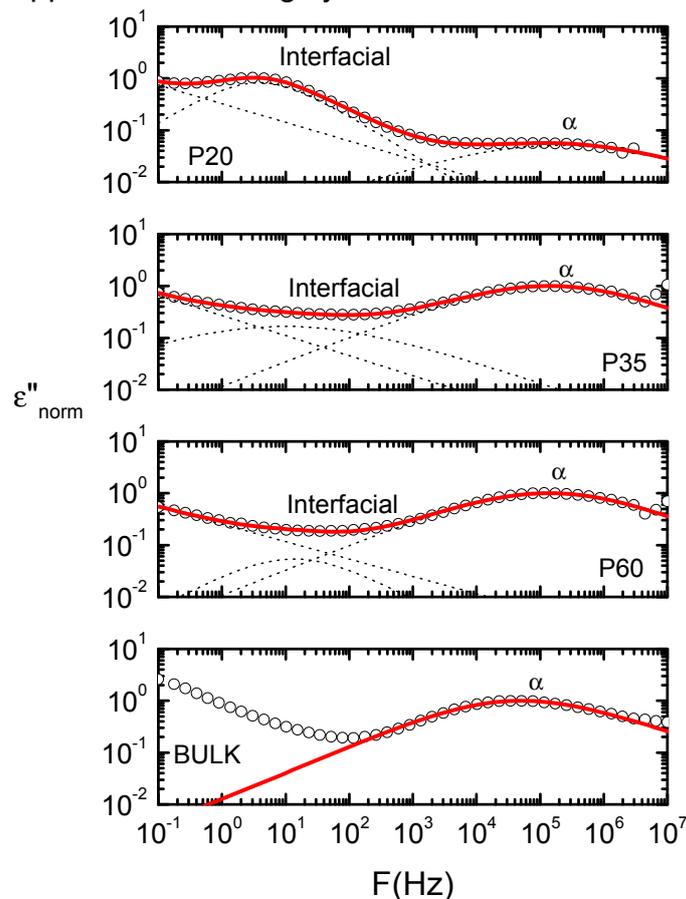
² S. Lee et al., *Angew. Chem. Int. Ed.* **48**, 1467 (2009)

³ L.M. Molina et al., *Catalysis Today* (submitted)

Relaxation behaviour in nanorods and nanotubes of PVDF and PVDF based ferroelectric polymers

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Understanding the behavior of systems at the nanometer scale is a crucial step to the development of nanotechnology. Dramatic finite size effects can be observed on the polymer dynamics as well as on the crystallization behavior. PVDF is a semicrystalline polymer which can be infiltrated in AAO templates producing either nanotubes or nanorods depending on the pore size and on the conditions of the infiltration. We present how confinement affects the relaxational behaviour and the ferroelectric to paraelectric transition in nanorods of PVDF and PVDF based ferroelectric copolymers. The nanorods have been prepared by infiltration into AAO templates with pore diameter in the range of 20 to 400 nm. We observed a strong deviation in the relaxation behavior of the amorphous phase of poly(vinylidene fluoride) (PVDF) embedded within self-ordered porous aluminum oxide templates as compared to that of the bulk, resulting in the appearance of a highly constrained relaxation.



Dielectric losses as a function of frequency PVDF sample under different confinement

Velocity map imaging of photoelectrons in pump-probe experiments combining synchrotron and laser radiation

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Velocity map imaging has been used to measure the photoelectron angular distributions (PAD) of electrons emitted from polarised rare gas atoms. Aligned ensembles of Rydberg atoms are prepared by photoexcitation using linearly polarised synchrotron radiation from the GasPhase beamline at the Elettra synchrotron source. The subsequent states were photoionised by linearly polarised laser light and the resulting “cloud” of photoelectrons was projected onto a position sensitive detector¹. Analysis of the resulting image (see for example figure 1) allowed the PAD of the emitted electrons to be characterised by the β_2 and β_4 parameters of the following formula:

$$I(\theta) = \frac{\sigma}{4\pi} [1 + \beta_2 P_2(\cos \theta) + \beta_4 P_4(\cos \theta)]$$

These asymmetry parameters are related to the radial matrix elements and phase differences of the outgoing electron waves in the continuum.

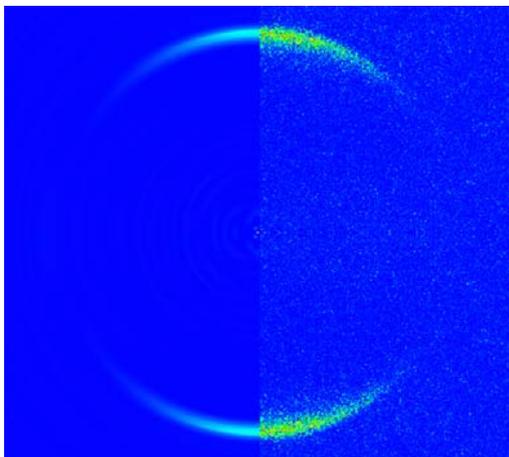


Fig.1: On the right side is the raw photoelectron image obtained following photoionization of the synchrotron prepared He 1s3p Rydberg states by a laser field with energy of 160 meV in excess of the ionization threshold. On the left hand side is the inverted image using the pBASEX method² from which the kinetic energy and angular distribution of the photoelectrons can be extracted.

In this work we studied the ionisation of several intermediate states in He, Ne and Ar for photoelectron energies from 20 to 100 meV. The geometry used in this experiment allows access to more parameters than revealed by previous methods³ thus providing a better description of the photoionisation event. The experimental results have been interpreted via an angular momentum analysis method as well as compared with the predictions of a quantum defect calculation.

¹ G. Cautero et al. *NIM A*, **595**, 447-459 (2008).

² G.A. Garcia et al. *Rev. Scient. Instr.* **75**, 4989-4996 (2001)..

³ Mitsuke K, Hikosaka Y and Iwasaki K *J. Phys. B:At. Mol. Opt. Phys.* **33**, 391 (2000)

Analysis of the formation of Metal/Organic Interfaces and Nanocontacts using Density Functional Theory

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The calculation of the electronic and structural properties of metal /organic nanocontacts and interfaces using conventional Density Functional Theory (DFT) presents important problems. One of them is the so called *energy gap problem of the organic materials*¹ DFT calculations yield HOMO/LUMO energy gaps that are significantly smaller than the transport gap measured experimentally. This is related to the fact that Kohn–Sham eigenvalues are not a proper representation of quasi-particle excitation energies and have to be corrected by the self-interaction energy of the corresponding wavefunction, to provide the appropriate molecule transport energy gap^{1,2}. Another problem is the poor description of weak interactions (e.g. van der Waals forces) in conventional DFT calculations.

In this talk we analyze the interaction of several organic molecules (TTF, TCNQ, C₆₀, bencene) with Au(111) surfaces and Au-tips. In our approach, we combine a DFT-LDA calculation of the structural and electronic properties of the system with an analysis of the interface barrier formation based on the Induced Density of Interface States model³. This allows us to determine in a simple way the self-interaction correction to the molecular orbitals levels, the transport energy gap and the metal/organic barrier height.

¹ F. Flores, J. Ortega and H. Vázquez, *Phys. Chem. Chem. Phys.* **11**, 8658 (2009)

² J.D. Sau *et al.* , *Phys. Rev. Lett.* **101**, 026804 (2008)

³ E. Abad, C. González, J. Ortega, F. Flores , *Organic Electronics* **11**, 332 (2010)

Self-consistent Bohmian description of laser-atom interactions

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The quantum-mechanical formulation of intense laser-atom interaction reduces to the well-known time-dependent Schrödinger equation (TDSE). Concurrent advances in methodology and computer performances have enabled sophisticated calculations which reproduced essential features such as above-threshold ionization¹ (ATI) and high-harmonic generation² (HHG) spectra. Nevertheless, bringing out the time-dependent dynamics of the total electron wavefunction is generally a non trivial task. Therefore, we are largely indebted to simplified models³, based on classical or semi-classical mechanics, for having improved our understanding of the laser-atom interaction by providing intuitive pictures in terms of electron trajectories. In this respect, a recent and great achievement consists of the so-called quantum orbit method⁴ (QOM), based on a Feynman's path-integral approach and using the Strong-Field Approximation⁵ (SFA) to determine electron trajectories beyond purely classical mechanics.

Nevertheless, the SFA, and related QOM, do not take the Coulomb forces into account and therefore do not apply in the multiphoton regime where intermediate excited states are involved in electron emission. Further, they are inadequate to the description of electron dynamics, and associated emission processes, close to the ionization threshold.

In this contribution, we thus consider the hydrodynamical formulation of TDSE, originally proposed by Bohm⁶, and its application to the description of one-electron laser-atom interactions. We specifically focus on a self-consistent hydrodynamical method that includes all external forces, beyond the SFA, and implement it to describe the electron dynamics in the (prototypical) one-dimensional H atom embedded in linearly polarized laser pulses. We explicitly prove that our self-consistent method yields electron densities, to which ATI and HHG spectra are directly related, as accurate as their standard TDSE counterparts. Further, the quantum trajectories shed light on the roles of the Coulomb, laser and self-consistent quantum fields in the time-dependent dynamics. The passage from multiphotonic to tunnel ionization regimes becomes particularly clear. Finally, the accuracy of both the QOM and Classical Trajectory Monte Carlo⁷ (CTMC) descriptions of harmonic generation is measured with respect to the Bohmian description.

¹ D. B. Milosevic *et al.*, *J. Phys. B* **39**, R203 (2006).

² C. Winterfeld *et al.*, *Rev. Mod. Phys.* **80**, 117 (2008).

³ P. B. Corkum, *Phys. Rev. Lett.* **71**, 1994 (1993).

⁴ P. Salières *et al.*, *Science* **292**, 902 (2001).

⁵ M. Lewenstein *et al.*, *Phys. Rev. A* **49**, 2117 (1994).

⁶ D. Bohm, *Phys. Rev.* **85**, 166 (1952); **85**, 180 (1952).

⁷ P. Botheron *et al.*, *Phys. Rev. A* **80**, 023402 (2009).

Molecular structure determination: a testing ground for high-level quantum-chemical computations

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An complete overview on various methodologies for determining molecular structure by means of quantum-chemistry as well as on the accuracy nowadays reachable will be presented.

Taking the coupled-cluster singles and doubles (CCSD) level augmented by a perturbative treatment of triple excitations (CCSD(T)) as starting point, emphasis will be given to extrapolation techniques as well as to inclusion of "minor" contributions, such as core-correlation effects, higher-excitation and relativistic effects.

The combination of experimental ground-state rotational constants with calculated vibrational corrections to determine reliable equilibrium geometries for polyatomic molecules will be also considered. Due to the computational contribution, these structures are usually referred to as "empirical", "mixed experimental/theoretical", or "semi-experimental". The comparison to pure ab initio structural determinations will be also discussed.

Illustrative examples, mostly for small to medium-sized molecules, will be presented.

Isotope effects in ion-atom collisions

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The study of the processes involved in ion-atom collisions are important in plasma physics, particularly in the fields of fusion research and astrophysics, where these collisions are used in both plasma diagnostic and plasma modeling. Among the various systems of interest, those involving protons (or isotopes) with beryllium are likely to be of the highest relevance because this metal is proposed as a first-wall material of the International Thermonuclear Experimental Reactor (ITER)^{1,2} and the tritium inventory is one of the crucial problems in the development of the reactor.

We have recently presented³ a detailed study of the proton collisions with Be in a wide energy range. The study was carried out by using the molecular method, where the collisional wave function, ψ , is expanded in a basis set of electronic states, ϕ , obtained from full configuration interaction (FCI) calculations carried out in a dense grid of values of the internuclear separation R . In that work, for impact energies below 0.6 eV/u, we find isotope effects larger than one order of magnitude for deuterium and two orders of magnitude for tritium, as can be appreciated in the figure. A simple two state model will be discussed in order to understand the physical origin of such a large isotopic dependence⁴.

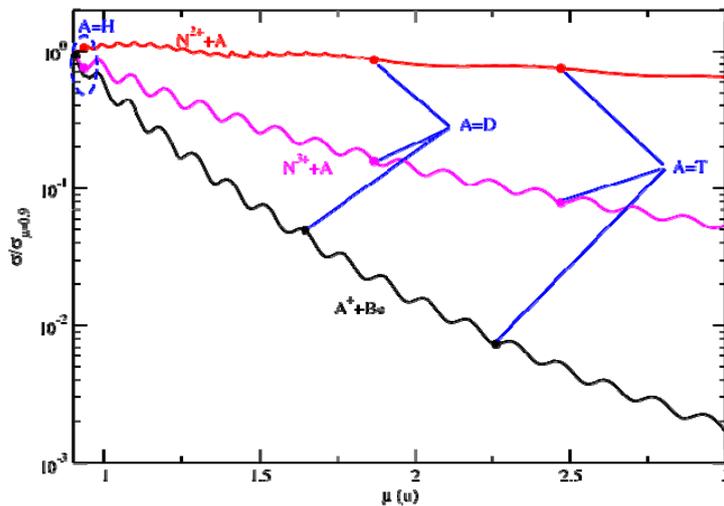


Figure 1. Isotopic dependence of the charge transfer cross section in collisions of $N^{2+}+A$, $N^{3+}+A$ and A^++Be , as a function of the reduced mass of the system. Here, A represents a fictitious hydrogen atom of variable mass. These results correspond to an impact energy of 25 meV/u.

¹ ITER Physics Expert Group on Divertor *et al.* Nuclear Fusion **39** 2391 (1999)

² K. Schmid, M. Baldwin, R. Doerner and A. Wilthner. Nuclear Fusion **44** 815 (2004)

³ P. Barragán, L. F. Errea, L. Méndez, I. Rabadán and A. Riera. J. Phys. B **41** 225202 (2008)

⁴ P. Barragán, L. F. Errea, L. Méndez, I. Rabadán. Submitted to Phys. Rev. Lett. (2010)

Simulation of folding processes of single-chain copolymers dilute solutions containing short chain branches.

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The crystallization process of macromolecular systems from both solution and molten state is a classical and fundamental problem in polymer physics. Unlike small molecular mass systems, polymers are unable to develop extensive single crystals. Instead, the bulk material organizes itself as a partially crystalline state, with alternating domains of amorphous and crystalline regions. In the present work, Langevin molecular dynamics (LMD) simulations have been performed in order to understand the role of the short chain branches (SCB) on the formation of ordered domains by cooling dilute solutions of ethylene/ α -olefins copolymer models. Three different long single-chain models (C_{2000}) with 0, 5 and 10 branches each 1000 carbons were selected. These models were equilibrated at high temperature ($T^*=13.3$) and cooling in steps of 0.45 until the final temperature ($T^*=6.2$) by running a total of 35×10^6 LMD steps. During the cooling process, global order parameter, torsion distribution, position of the branches and local-bond order parameter were calculated and monitored. The formation of order in the copolymers is affected by the amount of the SCB in the backbone of the polymer chain. First at all, the SCB move to the folding surface. Once the SCB are located near the folding surface the ordering starts to raise. The C_4 branches are excluded to the ordered domains. The crystallization temperature (T_c), crystallization fraction (α) and the density of the amorphous and ordered fractions was defined using the local-bond order parameter. All of them decrease as the number of branches increase. These facts fairly agree with experimental data available in the literature.

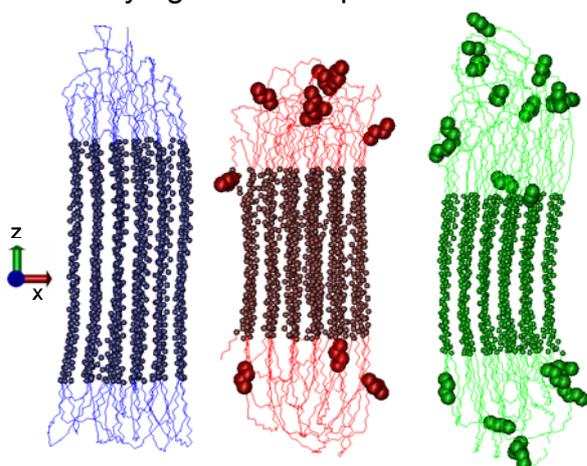


Figure 1. Selected geometries for the PE-00(blue), PE-05(red) and PE-10 (green) models showing the lamellar structure of the single-chain. Ball and stick stands for the ordered regions ($S_B(z) > 0.90$) and Van der Waals balls denote the branches.

Periodic driving of ultracold atoms in optical lattices

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We analyse how one can control the quantum states of ultracold bosons in an optical lattice using an oscillatory driving potential. We show that the tunneling and the localization properties of interacting bosons can be controlled by adiabatically turning on a fast oscillatory force. Our calculations are based on the exact solution of the time-dependent Schrödinger equation, using the Floquet formalism.

We consider the implications of our findings for larger systems and the possibility of controlling the phase diagram of disordered-interacting bosonic atoms.

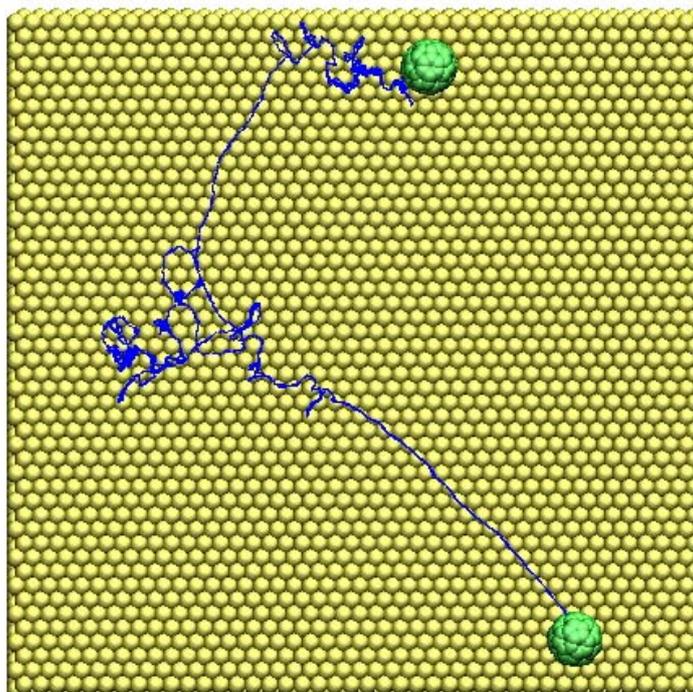
We also discuss how to induce finite momentum and generate a transient current.

Adsorption, Motion and Viscosity of Organic Molecules on Gold

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Physi- or chemisorbed monolayers of organic molecules on surfaces have great potential for practical applications that range from organic electronics, to sensing, to artificial noses. Initially, the molecules adsorb randomly. Over a certain period of time, they can form semi-ordered or ordered structures on the substrate surface, which can be either semiconducting or metallic. The high stability of Gold has made its surface very attractive for these processes. The adsorption of thiols on Au(111) is a classic example that has generated the well-known field of the self-assembled monolayers or SAMs. In this work we investigate with molecular dynamics 30 different molecules experimentally known to form ordered layers. We calculate a number of properties that range from their self-diffusion coefficients, by using the Green-Kubo relation (FACF) and the Einstein relation (MSD), to their viscosity via the Einstein-Stoke relation, to their entropy. We also determine the regime of the trajectories (diffusive, sub-/superdiffusive, Levy flight...). The trajectories of the thirty molecules share some common feature that can be used to explain the origin of the formation of the ordered layers.



Ultracold atom-ion collisions: Landau quantization and scattering resonances

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Ultracold atom-ion systems are a very promising system for the realization of quantum gates¹, applications in fundamental molecular physics² and the study of charged impurities in neutral Bose-Einstein condensates³. A detailed understanding of ultracold collisions in free space or in the presence of external fields is essential for all of these applications.

In this talk we present a theoretical study of ultracold atom-ion collisions in the presence of a uniform magnetic field. At low collision energies a magnetic field can modify drastically the translational motion of the ion which follows quantized cyclotron orbits, represented by Landau states in the plane orthogonal to the magnetic field. Due to this transverse confinement, the collision becomes effectively a one-dimensional process, in which an ion following a cyclotron orbit is reflected or transmitted across the target neutral atom. We present a rigorous theoretical framework for the calculation of reflection and transmission amplitudes within the close-coupling approach to time-independent scattering. Wigner threshold laws typical of 1D scattering are verified in our calculation. Our formalism applies to diffusion of particles with arbitrary axial angular momentum and lateral displacement of the target atom with respect to the cyclotron orbit centre.

We discuss collisions in different magnetic field regimes (weak, intermediate, strong) identified by the size of the cyclotron radius with respect to the typical range of the atom-ion interaction. The weak field limit can be mapped to the problem of motion in a waveguide, for which analytical solutions are known⁴. In the intermediate and strong field regimes the long-range interplay between the spherically symmetric potential and the axially symmetric magnetic field interaction has a strong quantitative and qualitative influence on the collision.

We show the occurrence of Feshbach resonances induced by the magnetic field in the three regimes considered. The resonance nature depends both on the magnitude of the applied magnetic field and on the axial angular momentum of the system. Such resonances exist independently of the spin of the colliding particles and could be used in practical applications to control the reflection and transmission of the ion across the target atom.

¹ H. Doerk-Bendig, Z. Idziaszek, and T. Calarco, "Atom-ion quantum gate", *Phys. Rev. A* **80**, 012708 (2010).

² Z. Idziaszek, T. Calarco, P. S. Julienne, and A. Simoni, "Quantum theory of ultracold atom-ion collisions", *Phys. Rev. A* **79**, 010702(R) (2009).

³ C. Zipkes, S. Palzer, C. Sias, and M. Köhl, "A trapped single ion inside a Bose-Einstein condensate", *Nature* **464**, 388 (2010).

⁴ M. Olshanii, "Atomic scattering in the presence of an external confinement and a gas of impenetrable bosons", *Phys. Rev. Lett.* **81**, 938 (1998).

Laser driven bond lengths with parabolic chirped pulses

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The Laser adiabatic manipulation of the bond (LAMB) method is a laser scheme that allows enlarging the characteristic bond length of a molecule by preparing a superposition of a bound electronic state and a dissociative electronic state. The word adiabatic refers here to the process by which one avoids increasing the (average) kinetic energy of the nuclei. This is achieved if the nuclear wave function stays basically on the ground state of the potential curve of the coherent superposition of electronic states, also called light-induced potential (LIP).¹ In order to significantly increase the bond length one needs to populate, in fact, almost invert the population, to predominantly anti-bonding orbitals. The bond distance is thus a function of the laser parameters (mainly the carrier frequency and pulse amplitude) which can be controlled externally.

Several LAMB schemes have been proposed in the literature which required at least two laser pulses and involved at least two excited electronic states.² In this work we propose an alternative simpler scheme which uses a single pulse with a non-linearly chirp (e.g. cubic optical phase). Control on the shape of the laser pulse is also relatively important. We show the underlying mechanism of this novel LAMB scheme and its robustness as well as the possible utility of the method.

¹ B. M. Garraway and K.-A. Suominen, *Phys. Rev. Lett.* **80**, 932 (1998)

² B. Y. Chang, H. Rabitz and I. R. Sola, *Phys. Rev. A* **68**, 031402 (2003)

Automatic Differentiation via operator overloading: a Fortran 95 implementation

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The need to calculate accurate derivatives of a multivariate function frequently arises in computational physics and chemistry. The most versatile approach to evaluate them by a computer, automatically and to machine precision, is via user-defined types and operator overloading. These features are provided by modern programming languages and effectively extend the capabilities of a compiler. The compiler can be taught to calculate the derivatives of any order, mixed or not, simultaneously with the value of a function, given only a minimally modified code implementing the function.

In my talk, an overview of the relevant features of Fortran 95 will be given and an implementation¹ of automatic differentiation based on them will be presented, along with examples. The speed of automatically evaluated derivatives is shown to be comparable to the hand-coded version in realistic cases. In terms of ease of computation and correctness, automatic differentiation via operator overloading turns out to be vastly superior to differentiation 'by hand', while much more accurate than any finite difference technique.

¹ S. Stamatiadis, R. Prosmiiti, S.C. Farantos, *Comput. Phys. Commun.* **127**, 343 (2000); S. Stamatiadis, *updated version in preparation*, (2010).

Electronic band-structure DFT analysis of phyllosilicates with metal-cation substitutions

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(c) Instituto de Física Fundamental, CSIC, Serrano 123, 28005 Madrid, Spain

Phyllosilicates are characterized by forming layer structures, they are one of the most frequent constituents of the Earth's crust and can be found on other planets, such as Mars [1]. Structures of phyllosilicates are based on two-dimensional layers of polyhedral networks: a two dimensional sheet based on SiO₄ tetrahedra. Other cations can substitute Si, producing different series of minerals. These tetrahedral sheets are linked in the unit structure to octahedral sheets, based on octahedra of XO₄(OH)₂ (X=Al³⁺, Mg³⁺, Fe³⁺ and Fe²⁺ but other cations occur in other species such as Ge⁴⁺ and Ga³⁺ [1]), forming a spread series of minerals. Moreover, depending on the octahedral site occupancy, two groups of phyllosilicates can be distinguished: the tri-octahedral series (full cation octahedral occupancy, with divalent cation, like Mg⁺² or Fe⁺²), and the di-octahedral series (where two out of every three octahedra are filled with trivalent cations such as Al³⁺ or Fe³⁺). Different charged cations of both series produced charged layers, which have to be compensated with interlayer cations.

Most of the phyllosilicates have an excellent performance as insulators, and so they have been widely used in industry. However, cation substitutions may alter their electrical behaviour, becoming a conductor [1,2]. The conductivity in biotite mica and tri-octahedral iron vermiculite and the influence of the composition in the conductivity were demonstrated and reported in biotite by Meunier et al. [3], and more recently in biotite and vermiculite by Ruscher et al. [4].

From the analysis of the band-structure calculated with Kohn-Sham density functional theory (DFT), it is possible to describe the electronic behaviour of phyllosilicates with the inconvenience of the systematic underestimation of the quasi-particle band gap, the so-called "band-gap problem", mainly rooted in the well-known self-interaction error in DFT [5-6].

In this work we present a DFT-based study of the influence of increasing the Fe^{2+,3+}, Ge⁴⁺ and Ga³⁺ content in the octahedral and tetrahedral sheet of tri-octahedral and di-octahedral phyllosilicates such as biotite, montmorillonite and kaolinite. The phyllosilicates electrical behaviour samples are analyzed as a function of the band-gap and the position of the Fermi level. DOS and PDOS analysis were also carried out to probe the influence of the metallic cation in the electronic properties of the samples. Finally, hybrid density functionals were employed (i.e., incorporating a fraction of the Hartree-Fock exchange) in order to correct the DFT band-gap and thus coming together with the experiment [7].

[1] F. Poulet, J.-P. Bibring, J. F. Mustard, A. Gendrin, N. Mangold, Y. Langevin, R. E. Arvidson, B. Gondet and C. Gomez, *Nature* **438**, 623-627(2005).

[2] G. Brown *Phil. Trans. R. Soc. Lond. A* **311**, 221 (1984).

[3] A. Meunier, J.F. Currie, M. R. Wertheimer and A. Yelon, *J. Appl. Phys.* **54**, 898 (1983).

[4] C.H. Rüscher and S. Gall, *Phys. Chem. Minerals* **24**, 365 (1997).

[5] A. Alkauskas, P. Broqvist, and A. Pasquarello, *Phys. Rev. Lett.* **101**, 046405 (2008).

[6] P. Rinke, A. Janotti, M. Scheffler, and C. G. Van de Walle, *Phys. Rev. Lett.* **102**, 026402 (2009).

[7] Elton A. S. Castro, João B. L. Martins, *International Journal of Quantum Chemistry* **103**, 550 (2005)

Oral Contributions

List of Oral Contributions

- P. Bargeño:** *"Subcritical temperature in Bose-Einstein condensates of chiral molecules"*
- M. Lara:** *"Reaching the cold regime: $S(^1D)+H_2$ open shell reactive collisions and the role of long-range interactions"*
- D. López-Durán:** *"ASPIN: An all spin scattering code"*
- S. López López:** *"High-dimensional system-bath quantum dynamics with selected-configurations wave functions"*
- J. S. Medina:** *"Molecular dynamics simulations of liquid water models: Temperature dependence of viscosities"*
- S. Monturet:** *"Electronic structure and dynamics of the vibrational relaxation of NO molecules scattered of a gold surface"*
- J. M. Oldham:** *"Cold state-selective ion-molecule reactions"*
- R. Pérez de Tudela:** *"Path-integral Monte Carlo on atomic clusters"*
- C. Sanz Sanz:** *"Dynamic Stark control of the photodissociation of IBr molecule"*
- Á. Valdés:** *"Translation-rotation energy levels of one H_2 molecule inside the small and medium cages of the structure H clathrate hydrate"*
- W. Unn-Toc:** *"Quantum dynamics at helium droplets"*
- Y. Wang:** *"Theoretical study on self-assembly of TCNQ adsorbed on Cu(100) surface"*
- A. Zanchet:** *" H_2 reactivity on gold clusters"*

Reaching the cold regime: S(¹D) + H₂ Open Shell Reactive Collisions and the Role of Long-Range Interactions

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Quantum reactive cross-sections for the collision of open shell S(¹D) atoms with *ortho*- and *para*-hydrogen, in the kinetic energy range 0–120 K (1K~ 9×10⁻⁵eV), have been calculated using the hyperspherical quantum reactive scattering method developed by Launay and Honvault¹. Short-range interactions, described using the *ab initio* potential energy surface by Ho *et al.*², were complemented with new accurate *ab initio* calculations of the long-range interactions. Both dispersion (~ R⁻⁶) and electrostatic quadrupole-quadrupole (~ R⁻⁵) contributions were considered. This allows the comparison with recent experimental measurements of rate constants (Rennes) and excitation functions (Bordeaux) for the title reaction at low temperatures³. The agreement is fairly good. The reactive behavior in the considered energy range can be understood on the average in terms of a classical Langevin (capture) model, where the centrifugal barriers determine the amount of reactive flux which reaches the barrierless transition state. Additionally, the structure of the van der Waals well provides temporal trapping at short distances thus allowing the system to find its way to reaction at some classically-forbidden energies. Interestingly, the cross-section for *para* hydrogen shows clearly oscillating features associated to the opening of new partial waves and to shape resonances which may be amenable of experimental detection.

¹ J. M. Launay and M. L. Dourneuf, *Chem. Phys. Lett* **169**, 473 (1990).

² T.-S. Ho, T. Hollebeek, H. Rabitz, S. D. Chao, R. T. Skodje, A. S. Zyubin, and A. M. Mebel, *JCP* **116**, 4124 (2002).

³ C. Berteloite, M. Lara, F. Dayou, S. D. L. Picard, A. Canosa, I. R. Sims, M. Costes, A. Bergeat, K. M. Hickson, C. Naulin, (Submitted to Science)

ASPIN: An all spin scattering code

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The field of cold molecules has recently experimented a rapid growth, both experimental and theoretical, mainly due to the spectacular results that have been achieved in the closely related area of Bose-Einstein condensates¹⁻³. We have previously presented the modified Variable Phase (VP) algorithm⁴, which was applied to the scattering process of a $^1\Sigma$ diatomic molecule with a 1S atom with an angular momentum state of $\Lambda=0$. Within the aim of extending that collision problem we present in this communication **ASPIN**⁵: a generalization of the code to open shell molecules. Now it is possible to consider the $^1\Sigma$, $^2\Sigma$, and $^3\Sigma$ diatomic target cases, thus covering the most common spin-rotation coupling schemes for diatomic species.

The main advantage of the modified VP propagator is that it is well suited for ionic systems, where a stronger interaction potential, in comparison with the neutral ones, is controlling the collision. This kind of propagator is specially faster than others due to its controlled reduction of the number of closed channels during the propagation of the solutions.

We will show two examples of application of **ASPIN**. The first example is the $\text{Li}_2(^1\Sigma_g^+)(^4\text{He})_N$ and $\text{Li}_2(^3\Sigma_g^+)(^4\text{He})_N$ clusters⁶, in which scattering calculations have contributed to clarify the dynamics of each complex. The second example is the isotopic effect in the rotational quenching of $\text{LiH}(X^2\Sigma^+)$ colliding with $(^1S)^{3,4}\text{He}$ ⁷.

We should remind that **ASPIN** is an open code published in *Computer Physics Communications*, and therefore can be used by any scientist.

¹ M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, E. A. Cornell, *Science* **279**, 198 (1995).

² C. C. Bradley, C. A. Sackett, J. J. Tollet, R. G. Hulet, *Phys. Rev. Lett.* **75**, 1687 (1995).

³ K. B. Davis, M. O. Mewes, M. R. Andrews, N. J. Van Druten, D. S. Durfee, D. M. Kurn, W. Ketterle, *Phys. Rev. Lett.* **75**, 3969 (1995).

⁴ R. Martinazzo, E. Bodo. and F. A. Gianturco, *Comput. Phys. Comm.* **151**, 187 (2003).

⁵ D. López-Durán, E. Bodo. and F. A. Gianturco, *Comput. Phys. Comm.* **179**, 821 (2008).

⁶ S. Bovino, E. Coccia, E. Bodo. D. López-Durán, and F. A. Gianturco, *J. Chem. Phys.* **130**, 224903 (2009).

⁷ D. López-Durán, M. Tacconi, and F. A. Gianturco, *Eur. Phys. J. D* **55**, 601 (2009).

High-Dimensional System-Bath Quantum Dynamics with Selected-Configurations Wave Functions

S. López-López and M. Nest

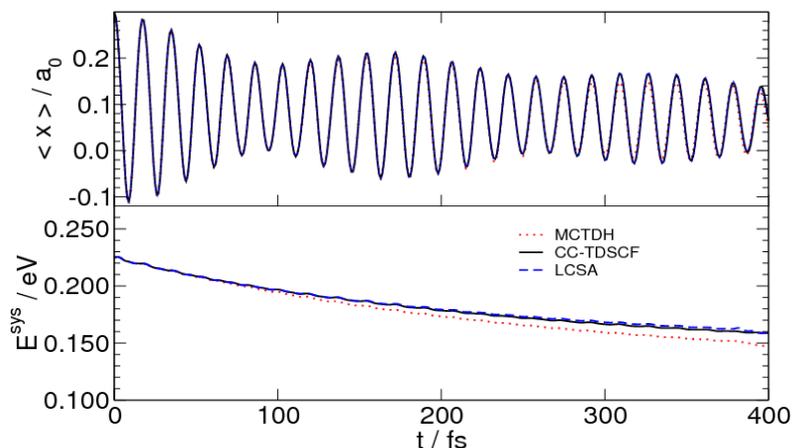
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Typical (sub)system-bath quantum dynamical problems are often well described by a selected-configuration, multiconfiguration expansion of the wavefunction of the whole system. For instance, the CC-TDSCF¹ and LCSA² methods, related to MCTDH³, use a simple Hartree product of bath single-particle-functions for each DVR state introduced in the Hilbert space of the subsystem:

$$|\Psi\rangle = \sum_{\alpha} C_{\alpha} |\xi_{\alpha}\rangle |\Phi_{\alpha}\rangle,$$

where $\{|\xi_{\alpha}\rangle\}$ denotes a DVR set for the subsystem coordinates, and $|\Phi_{\alpha}\rangle = \prod_{k=1}^f |\varphi_{\alpha}^k\rangle$ are the resulting *local* bath states, being f the number of bath degrees of freedom (DOF).

We have implemented and studied both schemes, also replacing the DVR states with eigenstates of the subsystem Hamiltonian, i.e. adopting an energy-local representation for the subsystem. We have found that stable and accurate results are obtained for a number of quantum dissipative problems⁴, at a much lower computational cost than with MCTDH (namely, propagation times scale linearly with the number of bath DOF, instead of MCTDH's exponential behaviour). Furthermore, we have found that both methods give very similar results, thus suggesting that coherent-states are well suited to describe (local) bath states.



As a whole, present results highlight the importance of the system basis-set in the selected-multiconfiguration expansion of the wavefunction. They suggest that very accurate and yet computationally cheap methods may be simply obtained from CC-TDSCF/LCSA by letting the subsystem states be variationally optimized.

¹ S. López-López and M. Nest, *J. Chem. Phys.* **132**, 104103 (2010)

² R. Martinazzo, M. Nest, P. Saalfrank, and G. F. Tantardini, *J. Chem. Phys.* **125**, 194102 (2006)

³ M. H. Beck, A. Jäckle, G. A. Worth, and H.-D. Meyer, *Phys. Rep.* **324**, 1 (2000)

⁴ S. López-López, R. Martinazzo and M. Nest, *J. Chem. Phys.* (submitted)

Electronic structure and dynamics of the vibrational relaxation of NO molecules scattered off a gold surface

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We examine the breakdown of the Born-Oppenheimer approximation in the framework of molecule-surface interaction. A vibrating NO molecule scattered from a gold surface can exchange energy with the electronic degrees of freedom of the metal (electron-hole pair creation), thus lowering its vibrational energy¹. The significant observed loss of energy, around 1.5 eV or 7 to 8 vibrational quanta, shows that close to the surface the nonadiabatic effects are important and eventually govern the dynamics of the scattering process. To understand this phenomenon, we first perform periodic DFT calculations to obtain a potential energy surface. Additionally, perturbative coordinate-dependent vibrational lifetimes² are computed with the help of the *ab initio* wavefunctions. Finally, we use a simple colinear model to simulate the approach of the NO molecule to the surface: this time-dependent quantum mechanical approach based on the reduced density-matrix³ includes the dissipative term responsible for the vibrational relaxation of NO. This is achieved with the help of Lindblad operators⁴.

¹ N. H. Nahler, J. D. White, J. La Rue, D. J. Auerbach, A. M. Wodtke, *Science*, **321**, 1191 (2008); J. D. White *et al.* *Nature*, 433, 503 (2005); H. Huang *et al.* *Science*, **290**, 111 (2000)

² N. Lorente, M. Persson, *Faraday Discuss.* **117**, 277 (2000)

³ P. Saalfrank, R. Kosloff, *J. Chem. Phys.* **105**, 2441 (1996)

⁴ P. Saalfrank, *Chem. Rev.* **106**, 4116 (2006)

Cold State-Selective Ion-Molecule Reactions

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Progress towards studying low-energy ion-molecule reactive collisions using a combined ion trap and Stark decelerator apparatus is presented. Ensembles of atomic and molecular ions are trapped in a linear radiofrequency ion trap and slowed by laser- and sympathetic-cooling, forming an ordered-structure known as a “Coulomb crystal.” These structures last for many hours under UHV conditions and are a sensitive probe for cold reactions, allowing almost unit-efficiency in detection of reactive collisions.¹ Atomic calcium ions are observed by detection of fluorescence emitted during laser cooling. Fluorescence images recorded during reaction experiments are in excellent agreement with results from molecular dynamics simulations and in collaboration allow an accurate determination of ion temperatures and numbers.

Neutral polar molecules are produced at low velocities using the Stark deceleration technique of Meijer and co-workers and subsequently focussed into the centre of the ion trap, where the Coulomb crystal acts as a target for the molecules. Previous studies in Oxford of cold ion-molecule reactions have used an electrostatic quadrupole guide velocity selector, providing a translationally cold but rotationally hot flux of molecules.² Stark deceleration is intrinsically quantum state-selective and can be used to produce molecular beams with tuneable velocities and high energy resolutions.³ We report progress on a proof-of-principle charge-exchange reaction between sympathetically-cooled Kr^+ ions and Stark-decelerated ND_3 .

¹ S. Willitsch et al. *Phys. Rev. Lett.* **100**, 043203 (2008)

² M. T. Bell et al. *Faraday Discuss.* **142**, 73 (2009)

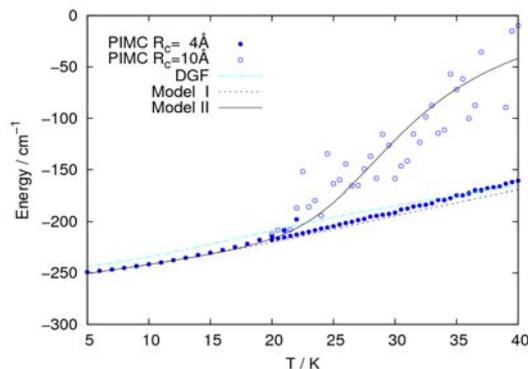
³ C. E. Heiner et al. *Phys. Chem. Chem. Phys.* **8**, 2666 (2006)

Path Integral Monte Carlo calculations on atomic clusters

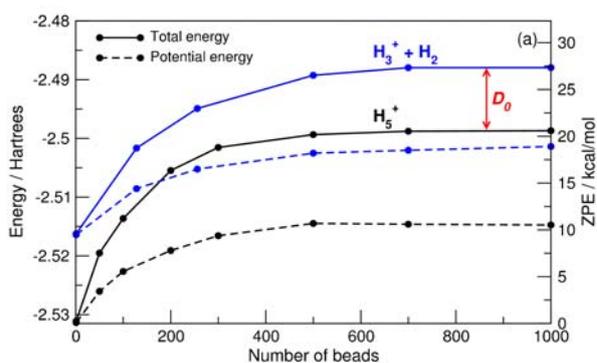
R. Pérez de Tudela, M. Márquez-Mijares, P. Barragán, T. González-Lezana, R. Prosimi, O. Roncero, S. Miret-Artés, P. Villarreal and G. Delgado-Barrio

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Classical and quantum Path Integral Monte Carlo (PIMC) calculations have been performed to study two different kinds of atomic clusters. In the first part, heavy-atom microcluster Ar_3 in the temperature range from 1 K to 40 K was studied¹. PIMC results using different confinement radii were compared with other theoretical approaches, such as Distributed Gaussian Function (DGF) method² and simple analytical models involving either the discrete (Model I) or both the discrete and continuum spectrum (Model II) (see top figure). The main conclusion is that the influence of the continuum is determinant in the dynamics of small clusters beyond a critical temperature.



In the second part we focus our research on ionic hydrogen clusters, which are relevant in astrophysics due to their presence in interstellar clouds and atmospheres of jovian planets³. Structural and energetic properties of H_5^+ and its fragments H_3^+ and H_2 were calculated at low temperature⁴, via "on fly" *ab initio* path integral Monte Carlo calculations, employing a DFT functional specially designed for hydrogen-only systems. This approach allows us to obtain a low computational cost surface that describes all the particular features of H_5^+ ⁵. In this way we achieve fully converged *ab initio* PIMC results for the thermostatics of the cluster. Of particular relevance are the vibrational zero-point energies (ZPE) and states and the dissociation energy



D_0 (see bottom figure). Results will be discussed and compared with other calculations and experimental measurements⁶.

- ¹ R. Pérez de Tudela *et al.* *J. Chem. Phys.* submitted (2010)
- ² M. Márquez-Mijares *et al.* *J. Chem. Phys.* **130**, 154301 (2009)
- ³ B. J. McCall and T. Oka *Science* **287**, 1941 (2000)
- ⁴ R. Pérez de Tudela *et al.* *J. Chem. Phys.* submitted (2010)
- ⁵ P. Barragán *et al.* *J. Chem. Phys.* submitted (2010)
- ⁶ T. C. Cheng *et al.* *J. Phys. Chem. Lett.* **1**, 758 (2010)

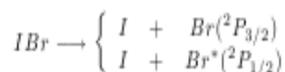
Dynamic Stark control of the photodissociation of IBr molecule

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In the last decade one of the main goals in chemistry, either experimental or theoretical, has been the control of chemical reactions. The majority of this control lies in the weak-field limit, in which the light-matter interaction can be taken as a perturbation on the Hamiltonian. The light-matter interaction only provides coupling to change the population of states. In the intermediate regime, the one we are interested in, the field is strong enough that the perturbation theory no longer applies, but not strong enough to produce ionisation. In this limit the electric field is able to change the potential energy surfaces (PES).

Modern ultrafast laser pulses are on the time scale of chemistry itself, so precise control over the shape and delay of these pulses offers access to different portions of the PES. The Stark effect is produced when a static field alters molecular states. When the field applied is time dependent the process is known as dynamic Stark effect (DSE). Of particular interest is the non-resonant dynamic Stark effect (NRDSE), in which the time dependent field is unable to effect a one-photon excitation. The laser pulse is used to shape the PES. The control of the photodissociation of IBr using NRDSE has been demonstrated by Stolow and coworkers^{1,2}. Non-adiabatic processes as internal conversion and intersystem crossing entail charge rearrangements that occur along a reaction path at the intersections of PES. Chemical branching ratios in non-adiabatic processes are very sensitive to the intersection geometry, and therefore the dynamic modification of these processes is an important application of the NRDSE. The photodissociation of IBr is initiated by absorption of a visible photon, exciting the system from the ground electronic state, $1^1\Sigma^+$ to the excited state $1^3\Pi_{0+}$. The non-adiabatic intersection between states $1^3\Pi_{0+}$ and $1^3\Sigma^-$ leads to two dissociation channels (Fig.1)



The application of an infrared NRDSE field can be used to modify the curve-crossing barrier at a specific time, promoting the yield of one dissociation channel over another (Fig. 2).

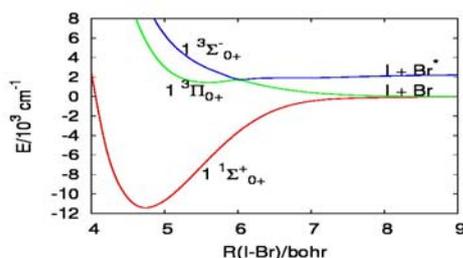


Figure 1: Ground and two intersecting excited states

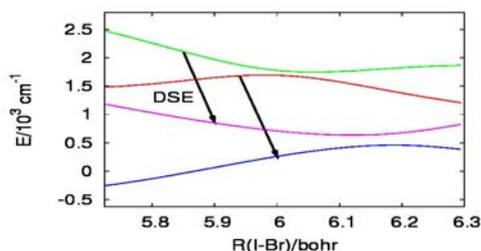


Figure 2: DSE of crossing intersection

The theoretical study done so far for IBr molecule will be presented here. We have calculated the several potential energy curves correlating with both spin-orbit states of I and Br ($^2P_{1/2}$ and $^2P_{3/2}$) for different intensities and orientations of the field. The potential energy and dipole curves were computed using the Electronic Nuclear Born-Oppenheimer (ENBO) approximation included in MOLPRO³. Those curves were used for the dynamics calculations using the Multi Configuration Time Dependent Hartree (MCTDH)⁴ package.

[1] B.J. Sussman, M.Y. Ivanov and A. Stolow, Phys. Rev. A, 71, 051401 (2005)

[2] B.J. Sussman, D. Townsend, M.Y. Ivanov and A. Stolow, Science, 314, 278 (2006)

[3] www.molpro.net

[4] G.A.Worth, M.H.Beck, A.Jackle, and H.-D.Meyer. The MCTDH Package, Version 8.2, (2000),

University of Heidelberg, Heidelberg, Germany.

Quantum dynamics at helium droplets

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For the last few decades, helium droplets have been constituting an active theoretical and experimental field of research thanks to their remarkable properties. Indeed, experiments on molecular systems embedded or on the surface of helium droplets have demonstrated superfluidity at low temperature (0.38K) and a high heat conductivity that make these doped droplets a very interesting solvent to study molecular dynamics.

Our aim is to describe the behaviour of these many-body systems at a microscopic level and to reproduce results of recent time resolved experiments. To this end, we have developed a real-time quantum dynamics method which can take into account the bosonic nature of ^4He by adding exchange symmetry and correlations.

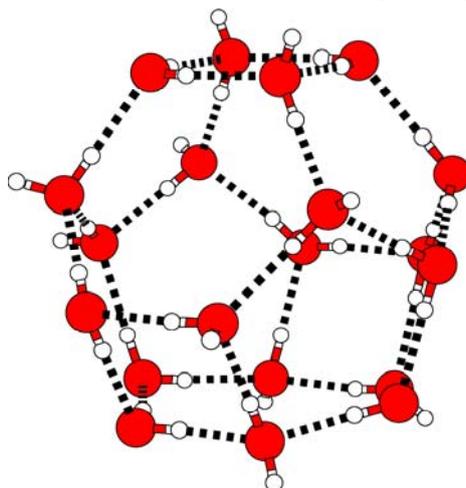
Our approach is based on the Multi-Configuration Time-Dependent Hartree (MCTDH) method. We will present the details of the model, and our first results on simple few-particle systems.

Translation-rotation energy levels of one H₂ molecule inside the small and medium cages of the structure H clathrate hydrate

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Clathrate hydrates are formed when water and 'guest' molecules come into contact under high pressure and low temperature conditions [1]. This kind of materials has generated a great interest because of their potential as hydrogen storage material. We report quantum dynamics calculations of the ro-vibrational energy levels of the hydrogen molecule inside the small and medium cage of the structure H clathrate hydrate [2], which are treated as rigid. The calculations are performed using the multiconfiguration time-dependent Hartree (MCTDH) method [3]. Some low-lying states are computed for both *para*-H₂ and *ortho*-H₂ by block improved relaxation. Contrary to the single occupancy, the inclusion of more than one H₂ molecule in the cages gives high positive ground state energies giving an indication that double occupancy is highly unfavourable.



[1] T. A. Strobel, K. C. Hester, C. A. Koh, A. K. Sum, E. D. Sloan Jr., *Chem. Phys. Lett.*, **478**, 97-109, (2009)

[2] Á. Valdés and G.-J. Kroes, *J. Chem. Phys.* (to be submitted)

[3] G. A. Worth, M. H. Beck, A. Jäckle and H.-D. Meyer, The MCTDH Package, Version 8.4 (2007). <http://mctdh.uni-hd.de>

Theoretical study on self-assembly of TCNQ adsorbed on Cu(100)

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(k) Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, Switzerland

The interface between tetracyano-*p*-quinodimethane (TCNQ) and copper is considered a model system for the interfaces between the strong electron acceptors usually involved in organic light-emitting diodes or organic solar cells and the metallic contacts. Recent STM and LEED experiments have congruously observed self-organized patterns of TCNQ molecules adsorbed on Cu(100) surface [1]. Our DFT studies show that charge-transfer between the adsorbate and the substrate plays a key role in the self-assembly of TCNQ on Cu(100), which is consistent with XPS and NEXAFS experiments¹.

The calculated adsorption energy is 2.23 eV for an isolated molecule on the surface, indicating a strong chemisorption. The binding energy for the complete monolayer is slightly larger, 2.35 eV per molecule, demonstrating further stabilization due to intermolecular interactions among the self-assembled molecules. The adsorbed TCNQ is no longer planar as in gas phase but has a bent conformation. The cyano groups are tilted towards the surface, confirmed by the measured bonding angle of 10.0–19.7° from NEXAFS analysis. The deformation of TCNQ at surface is enabled by the single-bond character of the Ph–CN bonds due to the charge-transfer of ~1.5 e⁻ from the surface to each molecule, supported by both calculations and XPS experiments. At the same time, substantial rearrangement of surface is observed; the copper atoms underneath nitrogen atoms are lifted from the surface plane by ~0.3 Å. The rearrangement of copper atom creates a stress field in such a way that the energy cost to lift a second atom out of its unperturbed equilibrium position is significantly reduced for the immediate neighbors of the already reconstructed copper atom bonded to the cyano group. This stress field makes the reconstructed copper atoms tightly grouped and energetically allows the copper atoms attached to cyano groups of different molecules to be in close proximity, and thus has a profound effect on the self-ordering of TCNQ on Cu(100) which could not be predicted on the basis of the gas-phase conformation of TCNQ. Its isotopic variants involving HD⁺ and D₂⁺ have been well investigated both experimentally^{1,2} and theoretically²⁻⁸. Besides being a test case of methods for ion molecule reactions, the above process is also important from the astrophysical point of view⁹⁻¹⁰. In order to explain the collisional outcomes of this reaction in various molecular beam experiments under different conditions, an accurate potential energy surface (PESs) is required.

¹ T.-C. Tseng, C. Urban, Y. Wang, et al, *Nature Chem.*, in press.

Posters

List of Posters

- E. Abad:** "Barrier formation and charging energy for metal/organic interfaces. From the monolayer to the single molecule limit: $C_{60}/Au(111)$ and $C_6H_6/Au(111)$ "
- J. R. Álvarez Collado:** "Efficient computational tools for calculating the quantum structure of large (1000-10000 electrons) un-localized macromolecular systems"
- D. Appaddo:** "Synchrotron THz absorption spectroscopy: A high-sensitivity technique to investigate molecular spectra"
- P. Bargaño:** "Subcritical temperature in Bose-Einstein condensates of chiral molecules"
- P. Barragán:** "A global potential energy surface for H_3^+ : A DFT approach"
- P. Barragán:** "A realistic DFT potential energy surface of H_5^+ cluster"
- M. Bartolomei:** "Theoretical studies for the O_2-N_2 intermolecular interaction: a new global potential energy surface"
- N. F. Aguirre:** "Interaction of He with a rutile $TiO_2(110)$ surface as a prototype case to include dynamical correlation in extended systems"
- A. Dorta-Urra:** "Potential energy surface and reactive dynamics of Au_2+H_2 "
- A. García-Vela:** "Femtosecond velocity map imaging experiments and wave packet calculations of CH_3I photodissociation in the A-band"
- T. González-Lezana:** "A dynamical study of the $O(^1D)+HCl$ reaction"
- L. González-Sánchez:** "Stereodynamics and mechanism of the $Cl+H_2$ reaction"
- Y. O. Guerrero:** "Theoretical study of the $HS(v',j'=1)+O_2(v''=0,j''1)$ reaction"
- M. Hernández:** "New ab initio potential energy surfaces for the oxygen dimer"
- R. Hernández Lamóneda:** "New ab initio potential energy surface and vibrational relaxation in $NO(v)+NO$ collisions"
- R. Hernández Lamóneda:** "Competition between electronic and vibrational predissociation dynamics of the $NeBr_2$ van der Waals complex: A model study"
- C. Illescas:** "Collisions of light ions with H_2O "
- D. López-Durán:** "Quantum solvent states of $(^4He)_N-Cs_2(^3\Sigma_u^+)$, $2 \leq N \leq 12$, clusters"
- M. Márquez-Mijares:** "A quantum-mechanical approach to study rovibrational spectra of molecular trimers"
- A. Martínez-Mesa:** "Influence of quantum effects on the physisorption of molecular hydrogen in model carbon foams"
- J. S. Medina:** "Molecular dynamics simulations of liquid water models: Temperature dependence of viscosities"
- J. Pérez-Torres:** "Attosecond XUV-IR laser pump-probe spectroscopy in H_2/D_2 "
- R. Prosmi:** "High-accurate potential surfaces and dynamics for $He-I_2$ "
- E. Quintas Sánchez:** "Eley-Rideal recombination of nitrogen on Tungsten(100)"
- A. Rivero-Santamaría:** "Dynamical study of the $O(^1D)+H_2(v_i=0,j_i=0) \rightarrow OH(X^2P, v_f, j_f)$ reaction using the Mean Potential Phase Space theory"
- LI. Uranga Piña:** "Quantum dynamics and ultrafast relaxation of photoexcited $NO(A^2S^+ \leftarrow X^2P)$ in cryogenic rare gas matrices"
- L. Velilla:** "Long range interaction inclusion in the HeH_2^+ potential energy surface"
- A. Zanchet:** " H_2 reactivity on gold clusters"

Barrier Formation and Charging Energy for Metal/Organic Interfaces. From the Monolayer to the Single Molecule Limit: $C_{60}/Au(111)$ and $C_6H_6/Au(111)$

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New electronic devices, like OLEDs, based on organic materials have already appeared in the market. The performance of these devices depends critically on the energy barriers created between different organic and metal layers. These are determined by the relative position of the molecular levels across the metal/organic (M/O) or the organic/organic (O/O) interfaces^{1,2}.

Molecular level alignment at M/O junctions has been extensively studied^{1,2}. The Schottky-Mott rule, based on the vacuum level alignment, has been disproved by the substantial interface dipole exhibited by many M/O junctions. In order to explain the alignment several models have been proposed. Of particular interest is the Induced Density of Interface States (IDIS) model¹, that is based on the tendency of the Charge Neutrality Level (CNL) of the organic material to align with the metal Fermi level due to the charge transfer between the two materials. In this work we combine a DFT calculation of the structural and electronic properties of M/O interfaces with an analysis of the interface barrier formation based on the IDIS model¹. It is well-known that in these systems it is necessary to go beyond standard DFT to properly describe the HOMO-LUMO gap and thus obtain a correct description of the electronic structure of the interface. Our analysis allows us to determine the charging energy (U^{eff}) of the molecule at the interface, correct the DFT transport energy gap and obtain a realistic metal/organic barrier height³. This method has been applied to the $C_{60}/Au(111)$ and benzene/ $Au(111)$ interfaces for various coverages, from the monolayer to the single molecule limit. Realistic benzene-gold distances have been calculated including the Van der Waals interaction⁴ in the DFT calculations of the interface.

¹ F. Flores, J. Ortega, H. Vázquez, *Phys. Chem. Chem. Phys.* **11** 8658 (2009)

² D. Cahen, A. Kahn and E. Umbach, *Materials Today* **8** 32 (2005)

³ E. Abad, C. González, J. Ortega, F. Flores, *Org. Electron.* **11** 332 (2010)

⁴ Y. J. Dappe, M. A. Basanta, F. Flores, J. Ortega, *Phys. Rev. B* **74** 205434 (2006)

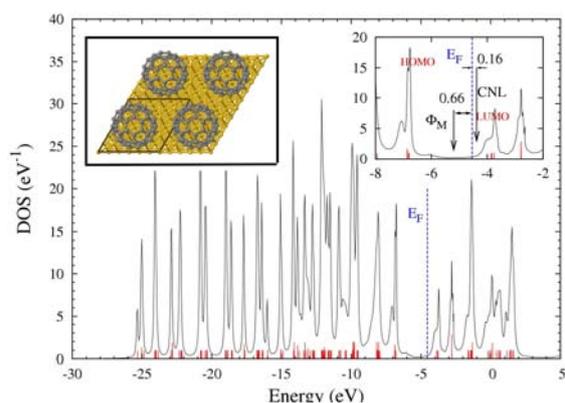


Figure 1: DOS projected on the C_{60} orbitals for the $C_{60}/Au(111)$ $2\sqrt{3}\times 2\sqrt{3}$ $R30^\circ$ monolayer shown in left inset. Right inset: Enlarged image for the area around the Fermi Level, showing HOMO, LUMO and CNL of the molecule, Φ_M of non-interacting gold surface and Fermi Level (E_F) of the system. Note that $E_F - \Phi_M$ is the IDIS potential Δ^{IDIS} . The molecular levels for the C_{60} neglecting interaction with surface are shown as red vertical lines.

Efficient computational tools for calculating the quantum structure of large (1,000-10,000 electrons) un-localized macromolecular systems

J. R. Álvarez Collado

Química Física Aplicada, Universidad Autónoma de Madrid, Spain

I have designed efficient software for calculating the quantum properties of large molecular systems.

The method works to restricted SCF semi-empirical level.

A calculation for a system having 10,000 electrons, 1000 of them unpaired, can be done in 10 hours in a PC.

The quantum properties of any hetero-aromatic hydrocarbon with 500 atoms can be obtained, in one PC minute, directly from its chemical formula. It is the only input required.

Synchrotron THz Absorption Spectroscopy: a high-sensitivity technique to investigate molecular spectra.

Dominique Appadoo
Australian Synchrotron, 800 Blackburn Rd, Clayton, Australia

A THz/Far-IR beamline with high spectral resolution capabilities has been constructed at the Australian Synchrotron. The THz/Far-IR beamline is coupled to a Bruker IFS125HR FT spectrometer equipped with a variety of optical components covering the spectral range from 10 to 1000 cm^{-1} ; this instrument can offer an optimum unapodized resolution of 0.00064 cm^{-1} (or ~ 20 MHz). Experiments from a variety of fields such as atmospheric and astrophysical science, geology, as well as biology and biomedicine have been successfully conducted at the beamline.

A range of instruments have been installed in order to accommodate the scientific requirements of Users: two room-temperature gas cells with multiple-pass optics, one for non-reactive species and one coupled to a furnace to study reactive species; there is also a multiple-pass gas cell which can be cooled to liquid N₂ and liquid Helium temperatures in order to study *supercooled* gases and molecular clusters. Users also have access to a cryostat to study condensed phase systems, and a grazing incidence angle accessory to study thin films.

The synchrotron infrared light offers a S/N advantage over conventional thermal sources. This advantage varies to a great degree depending on the spectral region and the resolution required by the experiment. In this paper, the beamline and its performance will be presented as well as some of the interstellar molecular species studied, and future beamline developments that will be undertaken to enhance the performance in the THz region.

Subcritical temperature in Bose-Einstein condensates of chiral molecules

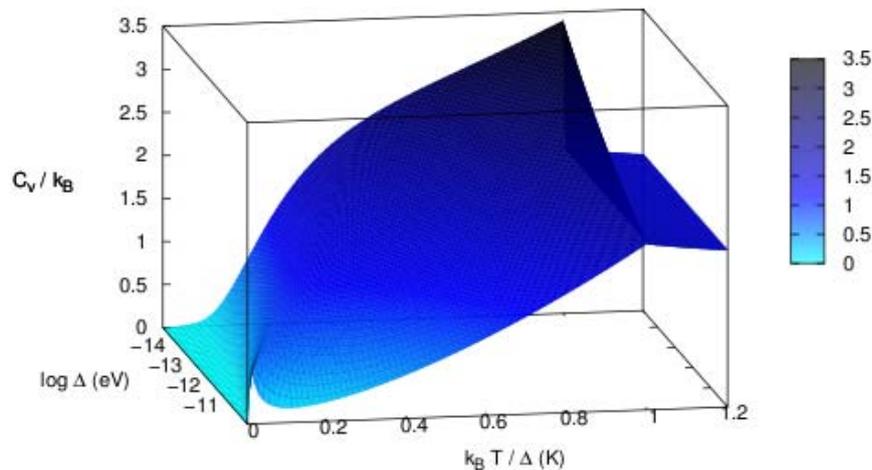
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^(c) *Departamento de Óptica, Avda. Complutense s/n, 28040 Madrid, Spain*

Bose-Einstein condensation of a sample of non-interacting chiral molecules leads to a non zero optical activity of the condensate and also to a subcritical temperature in the heat capacity. This is due to the internal structure of the molecule which, in our model, is considered as a simple two-state system, characterized by tunneling and parity violation. The predicted singular behavior found for the specific heat, below the condensation temperature, sheds some light on the existence of the so far elusive parity violation energy difference between enantiomers.



A global potential energy surface for H_3^+ : a DFT approach

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^(a) *Instituto de Física Fundamental, C.S.I.C., Serrano 123, 28006 Madrid, Spain*

A ground potential energy surface for the H_3^+ ion is obtained using density functional theory (DFT).¹ The potential was calculated using the B3(H) hybrid functional, that has been specifically parametrized for protonated hydrogen clusters. The surface has the appropriate topology to correctly describe equilibrium structures, linearization barrier and dissociation limits (see Fig. 1), and its features are compared with previous very-high accurate ab initio studies available, as well as with earlier and recent reported analytical potential energy surfaces. It is found that such approach produces a reasonable global potential, representing all aspects of ground-state H_3^+ .

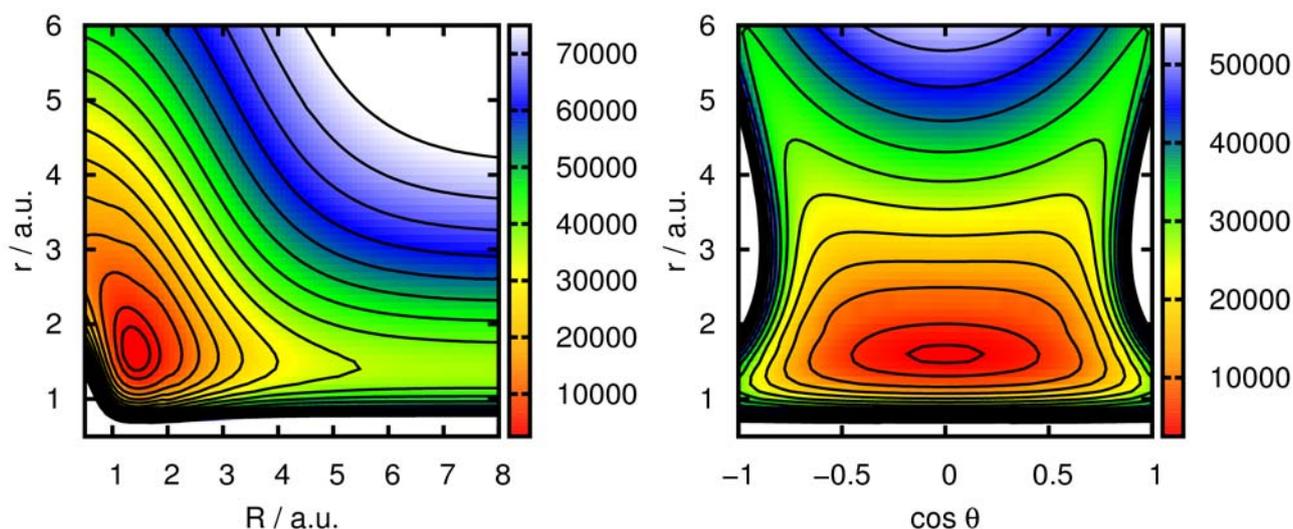


Fig. 1: Contour plots of the H_3^+ potential surface for $\theta=90^\circ$ (left panel) and $R=1.65$ a.u. (right panel). Contour intervals are of 5000 cm^{-1} and for energies of 2500 to 75000 and 55000 cm^{-1} respectively.

Such representations are in particular interesting for studying high-lying bound states of H_3^+ ,² and thus for a more accurate description of the PES, further improvement of the density functional employed in the present DFT calculations is proposed.

¹ P. Barragán *et al.*, *Inter. J. Quant. Chem.*, in press, DOI 10.1002/qua.22641 (2010).

² J. Tennyson, *Rep. Prog. Phys.* **57**, 421 (1995).

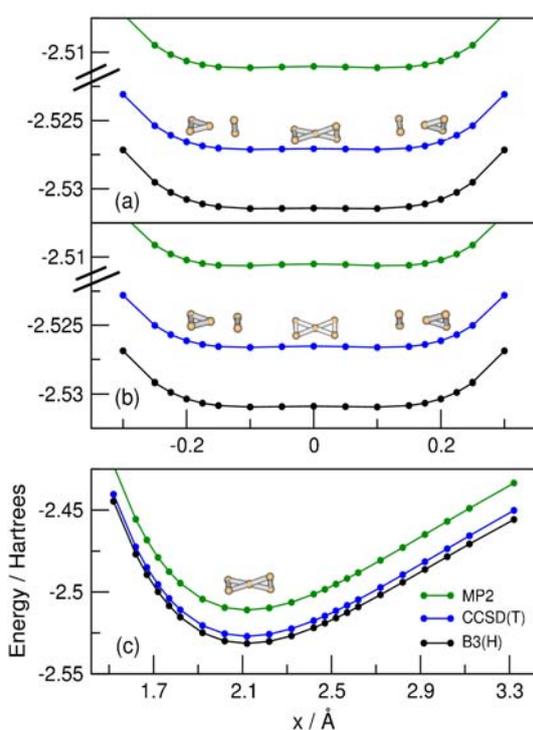
A realistic DFT potential energy surface of H_5^+ cluster

P. Barragán^(a), R. Pérez de Tudela^(a), R. Prosmi^(a), O. Roncero^(a), A. Aguado^(b),
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The potential energy surface of H_5^+ is characterized using density functional theory.¹ The potential hypersurface is evaluated at selected configurations employing different functionals, and compared with results obtained from *ab initio* CCSD(T) calculations. The lowest ten stationary points (minima and saddle-points) on the surface are located, and the features of the short-, intermediate-, and long-range intermolecular interactions are also investigated.



A detailed analysis of the surface's topology, and comparisons with extensive CCSD(T) results,² as well as a recent *ab initio* analytical surface,³ shows that DFT calculations using the B3(H) functional represent very well all aspects studied on the H_5^+ potential. These include the tiny energy difference between the minimum at 1- C_{2v} configuration and the 2- D_{2d} one corresponding to the transition state for the proton transfer between the two equivalent C_{2v} minima, and also the correct asymptotic behaviour of the long-range interactions. The calculated binding energy and dissociation enthalpies compare very well with previous benchmark coupled-cluster *ab initio* data, and with experimental data available.

Fig. 1: Optimal total energies for H_5^+ obtained at indicated levels. (a) The distance between the two H_2 monomers and the orientation of H_5^+ are fixed at the 2- D_{2d} and (b) 4- D_{2h} configurations. (c) The distance between the two H_2 varies, keeping fixed the proton in its middle for the 2- D_{2d} orientation.

Based on these results the use of such approach to perform first-principles molecular dynamics simulations could provide reliable information regarding the dynamics of protonated hydrogen clusters.⁴

¹ P. Barragán *et al.*, J. Chem. Phys., submitted (2010).

² R. Prosmi *et al.*, Theor. Chem. Acc., **106**, 426 (2001).

³ Z. Xie *et al.*, J. Chem. Phys., **122**, 224307 (2005).

⁴ R. Pérez de Tudela *et al.*, J. Chem. Phys., submitted (2010).

Theoretical studies for the O₂-N₂ intermolecular interaction: a new global potential energy surface

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The interaction between the two major components of the earth atmosphere, in their electronic ground state and considered as rigid rotors, has been obtained by means of *ab initio* electronic structure calculations. The SAPT(DFT) methodology, recently extended to treat open-shell monomers¹, has been employed to obtain interaction energies in a grid of 107 different dimer configurations. For each geometry a set of 19 intermolecular distances, covering the short range, well area and long range regions, has been used. A comparison with interaction energies obtained with the more computationally demanding RCCSD(T) method has been performed for selected dimer geometries. The multipole expansion for the electrostatic, dispersion and induction contributions needed for the extrapolation of the total interaction at larger intermolecular distances has been also obtained: for each monomer static and dynamic polarizabilities as well as permanent multipole moments have been calculated by using the CAS, MRCI and ACPF levels of theory.

The global potential energy surface, fitted with a spherical harmonic expansion, has been tested on experimental "hot" beam integral cross section² and second virial coefficient^{3,4} data. The lowest bound rotovibrational states and spectroscopic parameters for this weakly bound dimer have been also determined. A comparison with a previous experimentally derived potential energy surface⁵ is also presented.

¹ P. S. Zuchowski, R. Podeszwa, R. Moszynski, B. Jeziorski, K. Szalewicz *J. Chem. Phys.* **129**, 084101 (2008).

² B. Brunetti, G. Liuti, E. Luzzatti, F. Pirani, F. Vecchiocattivi *J. Chem. Phys.* **74**, 6734 (1981).

³ K. Fostiropoulos, G. Natour, J. Sommer, B. Schramm *Ber. Bunsenges. Phys. Chem.* **92**, 925 (1988).

⁴ J. H. Dymond, E. B. Smith, "The Virial Coefficients of Pure Gases and Mixtures", Clarendon Press, Oxford, (1981).

⁵ V. Aquilanti, M. Bartolomei, E. Carmona, F. Pirani *J. Chem. Phys.* **118**, 2214 (2003). P. J. Harvey *J. Chem. Phys.* **123**, 01234 (2008)

Interaction of He with a rutile TiO₂(110) surface as a prototype case to include dynamical correlation in extended systems

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This work is aimed at the calculation of the three-dimensional potential energy surface (PES) between a Helium atom and the rutile TiO₂(110) surface. Since the interaction of He with a metal-oxide surface is mainly dispersive, well depth being typically of about 10 meV¹, a high accuracy is required to obtain reliable potential energy surfaces. The inclusion of dynamic correlation (e.g., using the Møller-Plesset (MP2) or Coupled-Cluster (CCSD) levels of theory) is very important. Moreover, optimized basis sets need to be used to minimize the basis set superposition error (BSSE)², which otherwise is quite large. This study is motivated by an attempt at theoretical modelling of "soft-landing" processes on oxide surfaces through the embedding of targeted molecules and metal atoms (or bimetallic clusters) into He nanodroplets, as proposed by Vilesov, et al. in a previous experimental study³.

In the current work we show the results obtained for the interaction between a Helium atom and a TiO₂(110) surface, using the standard supercell-slab model⁴ and a Density Functional Theory-based (DFT) method (with the PBE functional) as available in the Crystal09 code⁷. An optimization of the basis set was necessary in order to minimize the basis set superposition error (BSSE) until ~ 3 cm⁻¹, estimated with the counterpoise method, which is quite large for standard basis sets (~ 400 cm⁻¹). The well depth obtained for the interaction between He atom and the Ti(5f) site on the surface (the most stable adsorption position), was estimated to be ~ 79 cm⁻¹ with an equilibrium distance of 3.2 Å. Finally, corrugation functions were calculated from the three-dimensional He-TiO₂(110) PES with associated amplitudes agreeing reasonably with those estimated in experimental measurements. We have also used a finite cluster model to simulate the extended system, by employing hydrogen atoms to saturate the dangling bonds (see e.g., Refs. 5-6). Hereafter, CCSD and the DFT-PBE treatments were applied to introduce the dynamical correlation, as implemented in the MOLPRO code. The DFT-PBE method shows results that match those obtained using Coupled-Cluster level of theory, independently of the cluster size.

¹ G. Benedek, G. Brusdeylins, V. Senz, J.G. Skofronick, J.P. Toennies, F. Traeger and R.Vollmer. *Phys. Rev. B.* **64**, 125421 (2009).

² M. P. de Lara-Castells, R. V. Krems, A. A. Buchachenko, G. Delgado-Barrio and P. Villarreal. *J. Chem. Phys.* **118**, 5098 (2003).

³ V. Mozhaykiy, M.N. Slipchenko, V. K. Adamchuk and A.F. Vilesov. *J. Chem. Phys.* **127**, 094701 (2007).

⁴ M. P. de Lara-Castells and J. L. Krause. *J. Chem. Phys.* **120**, 2182 (2001).

⁵ M. P. de Lara-Castells and J. L. Krause. *J. Chem. Phys.* **118**, 5098 (2003).

⁶ M. P. de Lara-Castells, A. O. Mitrushchenkov, O. Roncero, and J. L. Krause *Israel J. Chem Phys.* **45**, 59 (2005).

⁷ R. Dovesi, V. R. Saunders, C. Roetti, R. Orlando, C. M. Zicovich-Wilson, F. Pascale, B. Civalieri, K. Doll, N. M. Harrison, I. J. Bush, Ph. D'Arco and M. Llunell. See <http://www.crystal.unito.it/>

Potential Energy Surface and reactive dynamics of Au₂ + H₂.

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In this work we present a global Potential Energy Surface for the ground state of the Au₂ + H₂ reaction. The global potential is obtained by fitting ab initio calculation of the system, using Density Functional Theory in the Generalized Gradient Approximation with PW91 functional and relativistic pseudopotential for the gold atoms. The Minimum Energy Path of the fitting potential is compared with the corresponding molpro's¹ DFT-PW91 method, CCSD(T) and MRCI calculation, obtaining a good concordance. Preliminary results of Quasy-Classical Trajectory method are also presented.

¹ H.J. Werner and P.J. Knowles. *Package of ab initio programs*, 2008.

Femtosecond velocity map imaging experiments and wave packet calculations of CH₃I photodissociation in the A-band

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The velocity map imaging technique has been combined with femtosecond laser pulses to disentangle the time-resolved dynamics of the multichannel CH₃I photodissociation in the A-band. By using resonant detection, we have been able to clock the C-I bond rupture which involves non-adiabatic dynamics yielding ground-state I(²P_{3/2}) and spin-orbit excited I*(²P_{1/2}) and ground and vibrationally excited CH₃ fragments. The reaction times found for the different channels are directly related with the non-adiabatic dynamics of this multidimensional photodissociation reaction ¹. The experimental results have been compared with reduced-dimensionality wave packet calculations on available *ab initio* potential energy surfaces ^{2,3}. The model applied considers four degrees of freedom (4D) for CH₃I, namely the C-I dissociation coordinate, the I-CH₃ bending mode, the CH₃ umbrella mode, and the C-H symmetric stretch mode. An excitation femtosecond laser pulse (with FWHM=100 fs) centered at 266 nm has been employed in order to monitor the real time evolution of the system. The *ab initio* potential energy surfaces relevant to the photodissociation process in the maximum of the A-band (³Q₀ and ¹Q₁), the nonadiabatic coupling between them and the *ab initio* transition moments have been considered ^{2,3}. A detailed comparison between experimental and theoretical results and the agreements and discrepancies found will be presented and discussed.

¹ R. de Nalda, J. Durá, A. García-Vela, J. G. Izquierdo, J. González-Vázquez, L. Bañares *J. Chem. Phys.* **128**, 244309 (2008)

² D. Xie, H. Guo, Y. Amatatsu, R. Kosloff *J. Phys. Chem. A* **104**, 1009 (2000)

³ A. B. Alekseyev, H.-P. Liebermann, R. J. Buenker *J. Chem. Phys.* **126**, 234103 (2007)

Collisions of light ions with H₂O

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Ion collisions with H₂O molecules are relevant in radiation damage of biological system; in particular ionization processes yield low energy electrons which are responsible for the DNA strand breaking¹.

In this work, we present a study of the ionization and capture processes in collisions H⁺, He²⁺ and C⁶⁺ with water molecules. Single and total cross sections are obtained in the energy range $20 \text{ keV}/amu \leq E \leq 10 \text{ MeV}/amu$, in the framework of the CTMC method, using a three-center model potential to describe the target molecule. We have improved our CTMC method presented in a previous work² in order to better describe the anisotropy of the projectile-target interaction. The description of the electron initially bound to the water molecule, is performed using a microcanonical distribution³ for each orbital and with energy equal to the ionization energy of each of the four molecular orbital of the valence shell (2a₁, 1b₂, 3a₁, and 1b₁). Besides, we have considered 12 trajectory orientations of the projectile with respect to the molecular target to determine average total cross sections. To extract multielectronic probabilities from one-electron calculation, we have employed the Independent Event Model (IEVM), suggested in⁴ and used in several works for multiionization of atomic targets.

A detailed comparison with previous calculations and experimental results (see e. g.⁵ and references therein) will be presented at the Meeting. Also, we will analyse the asymptotic behaviour of the total ionization cross section and we propose scaling laws for capture and ionization cross sections.

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¹ B. Boudaïffa *et al.*, *Science* **287**, 1658 (2000)

² L. F. Errea *et al.*, *Phys. Rev. A* **76**, 40701 (2007)

³ R. Abrines and I. C. Percival, *Proc. Phys. Soc.* **88**, 873 (1966)

⁴ D. S. F. Crothers and R. McCarroll, *J. Phys. B* **20**, 2835 (1987)

⁵ C. Champion *et al.*, *J. Phys.: Conf. Series* **110**, 12010 (2008)

A dynamical study of the O(¹D)+HCl reaction

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The dynamics of the O(¹D)+HCl reaction has been recently [1] investigated at a 0.26 eV collision energy by means of quasi-classical trajectory (QCT) and statistical methods (both quantum mechanical (QM) [2] and trajectory versions [3]). Comparison with experimental studies reveals that the PSB2 surface [4] by Peterson and co-workers describe correctly differential cross sections and the velocity distributions of the departing Cl atom for the OH+Cl product arrangement. For the ClO forming channel, good agreement was found between the QCT cross sections and the statistical predictions.

Fully converged QM time-dependent wave packet (TDWP) reaction probabilities for a non-zero total angular momentum ($J > 0$), on the H₂ surface [5], are presented here for the first time. The dynamics of the O(¹D)+HCl → ClO+H reaction seems to be well described by the statistical approaches, whereas some quantitative deviations are observed with respect to the TDWP results for the OH+Cl product channel. The QCT probabilities in turn are in good accord with the QM values in all cases.

An energy dependent study of the reaction which includes integral and differential cross sections is presented in this communication.

[1] P. Bargeño *et al.*, *J. Phys. Chem. A* **113**, 14237 (2009)

[2] E. J. Rackham *et al.*, *Chem. Phys. Lett.* **343**, 356 (2001); E.J. Rackham *et al.*, *J. Chem. Phys.* **119**, 12895 (2003).

[3] F. J. Aoiz *et al.*, *J. Chem. Phys.* **126**, 161101 (2007); F. J. Aoiz *et al.*, *J. Chem. Phys.* **127**, 174109 (2007); **129**, 094305 (2008).

[4] M. Bittererova *et al.*, *J. Chem. Phys.* **113**, 6186 (2000); K. M. Christoffel and J.M. Bowman, *J. Chem. Phys.* **116**, 4842 (2002).

[5] T. Martínez *et al.*, *Phys. Chem. Chem. Phys.* **2**, 589 (2000)

Stereodynamics and mechanism of the Cl + H₂ reaction

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We present a quantum mechanical description of the Cl + H₂ (v=0, j=2) collisions stereodynamics at E_{coll}= 0.18, 0.68 and 1.18 eV. Both inelastic and reactive processes have been considered. Our methodology¹⁻³ is based on the analysis of the reactants intrinsic polarization that contains the directional preferences of the reaction and is exclusively determined by the dynamics. The moments describing this polarization, whose values have been evaluated from quantum mechanical scattering calculations, inform about the alignment and orientation of the H₂ orbital angular momentum when the reaction takes place and provide with valuable hints about the mechanism.

We have also studied the extend of the reaction control achievable by modifying the experimental polarization of the reactants². The idea is simple: a good (bad) matching between the intrinsic and the experimental polarizations leads to an increase (decrease) of the cross sections. Large changes in differential cross sections, both in value and in shape, are observed when different reagents preparations are used.

¹ M.P. de Miranda, F.J. Aoiz, L. Bañares and V. Sáez-Rábanos *J. Chem. Phys.* **111**, 5368 (1999)

² J. Aldegunde, M.P. de Miranda, J.M. Haigh, B.K. Kendrick, V. Sáez-Rábanos and F.J. Aoiz *J. Phys. Chem. A* **109**, 6200 (2005)

³ J. Aldegunde, J.M. Alvariño, B.K. Kendrick, V. Sáez-Rábanos, M.P. de Miranda and F.J. Aoiz *Phys. Chem. Chem. Phys.* **8**, 4881 (2006)

Theoretical study of the $\text{HS}(v',j'=1) + \text{O}_2(v''=0,j''=1)$ reaction

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We report a theoretical study of the title four-atom reaction for a wide range of translational energies, considering the reactants in the ground vibrational state and also in some vibrationally excited levels of the HS radical. All calculations have employed the quasi-classical trajectory (QCT) method and a reported double many-body expansion potential energy surface for ground electronic state of HSO_2 . Cross sections as well as specific rate constants for HS elimination are reported and compared with literature data for such processes. To account the zero-point energy problem in QCT calculations, an internal energy quantum mechanics threshold (IEQMT) criteria is used

New ab initio potential energy surfaces for the oxygen dimer

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The $O_2(^3\Sigma_g^-)$ - $O_2(^3\Sigma_g^-)$ dimer is of interest in atmospheric physics and chemistry, in condensed phase, and more recently, in low and ultralow temperature physics. As the electronic spin of the molecules is one, three different intermolecular potential energy surfaces (PESs) are generated with singlet, triplet and quintet multiplicities. We will report on the first global PESs (for rigid monomers) completely obtained from ab initio calculations¹, where the quintet state has been obtained at the RCCSD(T) level of theory² and the singlet and triplet ones are obtained by combining the RCCSD(T) quintet potential with multiconfigurational calculations of the singlet-quintet and triplet-quintet splittings³. In addition, the PESs are extrapolated at long range using accurate ab initio dispersion coefficients⁴.

The new PESs are checked against second virial coefficient data⁵, integral cross sections measured in rotationally hot effusive beams⁶ and overall, a satisfactory comparison is achieved. An even better agreement would be obtained if the computed PESs were slightly more attractive. A more critical test of the details of the interaction around the absolute minima is posed by spectroscopy^{7,8}. Bound state calculations of the dimer using the new PESs provide a very good agreement with rotationally resolved absorption spectra⁷ regarding the geometry of the ground vibrational state but differences appear for the dissociation energy. On the other hand, the singlet-triplet splitting compares quite well with measurements performed in a neon host a very low temperature⁸.

¹ M. Bartolomei, E. Carmona-Novillo, M. I. Hernández, J. Campos-Martínez, R. Hernández-Lamoneda, *J. Chem. Phys.*, submitted.

² M. Bartolomei, E. Carmona-Novillo *et al*, *J. Chem. Phys.* **128**, 214304 (2008).

³ M. Bartolomei, M. I. Hernández *et al*, *Phys. Chem. Chem. Phys.* **10**, 5374 (2008)

⁴ M. Bartolomei, E. Carmona-Novillo, M. I. Hernández, J. Campos-Martínez, R. Hernández-Lamoneda, *J. Computational Chem.*, submitted.

⁵ J. Dymond, E. Smith, *The Virial Coefficient of Pure Gases and Mixtures: a Critical Compilation* (Clarendon Press, Oxford, 1980)

⁶ V. Aquilanti, D. Ascenzi *et al*, *J. Am. Chem. Soc.*, **121**, 10794 (1999).

⁷ L. Biennier, D. Romanini *et al*, *J. Chem. Phys.* **112**, 6309 (2000).

⁸ J. Goodman and L.E. Brus, *J. Chem. Phys.* **67**, 4398 (1976).

New ab initio potential energy surface and vibrational relaxation in NO(v) + NO collisions

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A new ab initio Potential Energy Surface (PES) for the ground state of the NO-NO system has been calculated within a reduced dimensionality model. The characteristics of this PES are discussed and compared with theoretical and experimental results reported for NO-NO and other similar systems. The vibrational relaxation probabilities and rates were obtained using quantum scattering calculations and the results are compared with previous experimental studies for this and related systems. Our most significant results are: a) There is a strong dependence of the interaction potential with the NO stretching. This gives support to previous experimental spectroscopic studies[1] b) This study has shown that the vibrational relaxation for $v=1$ is much larger than in analogous systems and it isn't necessary to invoke special mechanisms such as non-adiabatic transitions to predict this unusual behavior[2]. c) For high vibrational states we predict a strong dependence of the rates on the vibrational quantum number as was observed experimentally by the Wodtke group[3], on the other hand there are important quantitative differences. We also analyzed the effect of a chemically bound intermediate complex which does not play a role at the values of v considered in the experiment but only at much higher energies. d) Another very interesting experimental observation is the negative temperature dependence of the rate constants[4,5]. We have analyzed whether such behavior can be explained on the basis of statistical arguments and the presence of many asymptotically degenerate electronic states.

- 1.- Brechignac, Ph, *et al*, *J. Chem. Phys.* **83**, 2064, 1985.
- 2.- E.E. Nikitin. *Theory of Elementary Atomic and Molecular Processes in Gases*. Clarendon, Oxford, 1974.
- 3.- Yang, X., Kim, E.H., Wodtke, A.M.; *J. Chem. Phys.* **96**, 5111, 1992.
- 4.- Rebelo da Silva, M., *et al*, *Chem. Phys. Lett.*, **91**, 135, 1982.
- 5.- James, P.L., Sims, I.R., Smith, I.W.M., *Chem. Phys. Lett.* **276**, 423, 1997.

Competition between electronic and vibrational predissociation dynamics of the NeBr₂ van der Waals complex: A model study

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Recently the predissociation lifetimes of the NeBr₂ (B) complex for several initial vibrational states ($10 \leq v \leq 20$) has been measured using time-resolved optical pump-probe spectroscopy[1]. In the vibrational interval studied the vibrational predissociation (VP) proceeds by the transfer of a single vibrational quantum, and the lifetimes are expected to decrease smoothly with increasing v , as predicted by the energy gap law. However, the experimental lifetimes show strong oscillations with v , which were attributed to the occurrence of electronic predissociation (EP) with several possible electronic states of Br₂, based on a Franck-Condon spectator model. In this work we clarify the nature of the electronic states that cause the predissociation and reproduce the experimental findings by performing full three-dimensional wavepacket calculations for the competition of vibrational and electronic predissociation. Model potential energy surfaces were used based on previous theoretical simulations of the VP dynamics on the B state [2] and on *ab initio* calculations on the related NeCl₂ system [3,4]. The strength of the electronic couplings is fit to achieve excellent agreement with experiment.

- 1.- Taylor, M.A. *et al*, *J. Chem. Phys.* **132**, 104309, 2010 .
- 2.- Roncero, O. *et al*, *J. Chem. Phys.* **115**, 2566, 2001.
- 3.- Hernández-Lamonedada, R., Janda, K.C., *J. Chem. Phys.* **123**, 161102, 2005.
- 4.- Bieler, C.R. *et al* , *J. Phys. Chem. A* **114**, 3050, 2010.

Quantum solvent states of $(^4\text{He})_N\text{-Cs}_2(^3\Sigma_u^+)$, $2\leq N\leq 12$, clusters

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Clusters and droplets of noble gases, mainly helium, have opened up a new field of research. In particular, the study of medium-size complexes has been motivated by striking phenomena like superfluidity¹. It is related with the completely different spectra of molecules embedded in this kind of clusters, depending on the bosonic or fermionic nature of the solvent: in the former case it is a well-defined profile, while in the latter any structure is lost.

In this work we study complexes formed by a diatomic Cs_2 molecule plus an ensemble of N ^4He atoms, with $N=2$ up to 12. In order to search for the ground state wave-function of the system we have employed a Hartree Quantum-Chemistry-like method², assuming adiabaticity in the diatomic stretch and decoupling of the diatomic rotation from the helium atoms^{3,4}. The PES's are described as a pair addition of all the He-He potentials plus anisotropic *ab initio* He- Cs_2 potential⁵.

We will show energetic and structural aspects of the clusters, trying to understand the arrangement of the impurity with respect to the helium cloud. Complementary path Integral Monte Carlo calculations at 1 K have also been carried out.

¹ S. Grebenev, J. P. Toennies, and A. F. Vilesov, **Science** 279, 2083 (1998).

² M. P. de Lara-Castells, D. López-Durán, G. Delgado-Barrio, P. Villarreal, C. Di Paola, F. A. Gianturco, and J. Jellinek, **Phys. Rev. A** 71, 033203 (2005).

³ D. López-Durán, M. P. de Lara-Castells, G. Delgado-Barrio, P. Villarreal, C. Di Paola, F. A. Gianturco, and J. Jellinek, **J. Chem. Phys.** 121, 2975 (2004).

⁴ D. López-Durán, M. P. de Lara-Castells, G. Delgado-Barrio, P. Villarreal, C. Di Paola, F. A. Gianturco, and J. Jellinek, **Phys. Rev. Lett.** 93, 053401 (2004).

⁵ R. Prosimiti, G. Delgado-Barrio, P. Villarreal, E. Yurtsever, E. Coccia, and F. A. Gianturco, **J. Phys. Chem. A** 113, 14718 (2009).

A quantum mechanical approach to study rovibrational spectra of molecular trimers.

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The study of rare gas clusters has been of great interest in Chemical Physics in recent years. These clusters offer an ideal scenario among atomic/molecular systems and continuum media (solids and fluids), making it possible to understand how properties of macroscopic systems arise from those of their atomic/molecular constituents, properties such as phase changes, equilibrium geometries or the superfluidity present in some bosonic aggregates.

A variational approach based in distributed Gaussian functions (DGF) to describe the interparticle distances has allowed a detailed study of the rovibrational spectrum of the argon trimer^{1,2,3}. The total Hamiltonian, H_{tot} , is assumed to be the sum of an exact vibrational ($J=0$) Hamiltonian, H_{vib} , and a rigid rotor-like part, H_{rot} , to describe rotation. The possible vibration-rotation interaction is then included by diagonalizing H_{rot} , in a basis formed by eigenstates of H_{vib} . Energy value and the corresponding assignment of a symmetry character have been compared with exact hyperspherical calculations^{2,3}. The calculation of higher value for total angular momenta ($J>40$) by means of this method has allowed compare estimations of the average energy in terms of the temperature with Path Integral Monte Carlo (PIMC) results^{4,5}.

Recent applications of this method on H_3^+ will be shown^(in this work) and compare with exact hyperspherical calculations⁶.

¹ I. Baccarelli, F. A. Gianturco, T. González-Lezana, G. Delgado-Barrio, S. Miret-Artés, and P. Villarreal, *Phys. Rep.* **452**, 1 (2007).

² M. Márquez-Mijares, T. González-Lezana, O. Roncero, S. Miret-Artés, G. Delgado-Barrio, and P. Villarreal, *Chem. Phys. Lett.* **460**, 417 (2008).

³ M. Márquez-Mijares, R. Pérez de Tudela, T. González-Lezana, O. Roncero, S. Miret-Artés, G. Delgado-Barrio, P. Villarreal, I. Baccarelli, F. A. Gianturco, and J. Rubayo-Soneira, *J. Chem. Phys.* **130**, 154301 (2009).

⁴ R. Pérez de Tudela, M. Márquez-Mijares, T. González-Lezana, O. Roncero, S. Miret-Artés, G. Delgado-Barrio, and P. Villarreal, *Few-Body Syst.* **45**, 237 (2009).

⁵ R. Pérez de Tudela, M. Márquez-Mijares, T. González-Lezana, O. Roncero, S. Miret-Artés, G. Delgado-Barrio, and P. Villarreal, *J. Chem. Phys.* (submitted 2009).

⁶ Alfredo Aguado, Octavio Roncero, Cesar Tablero, Cristina Sanz and Miguel Paniagua, *J. Chem. Phys.* **112**, 1240 (2000).

Influence of quantum effects on the physisorption of molecular hydrogen in model carbon foams

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The physisorption of molecular hydrogen in (5,5) zigzag carbon foams is investigated in the temperature range from 50K to room temperature. The study is carried out within the framework of the Density Functional Theory for quantum liquids at finite temperature introduced in PRE 80, 031603 (2009). It is shown that adsorption isotherms exhibit a weak dependence on the explicit incorporation of the bosonic exchange symmetry of hydrogen molecules. The relation between the microscopic structure of the hydrogen fluid and the calculated gravimetric and volumetric adsorption capacities is also addressed.

Molecular Dynamics Simulations of Liquid Water Models: Temperature Dependence of Viscosities

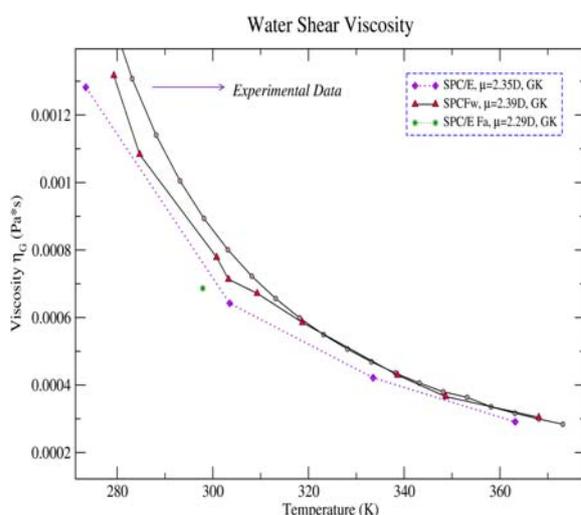
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Molecular dynamics simulations were carried out on a system of 256 water molecules in a rigid or flexible model at a series of temperatures between 273.32 and 368.13 K. The simulations were done at NVE ensemble to allow a proper use of Green-Kubo theory for assesment of transport coefficients.¹ Pressure tensor fluctuations, wich account for kinetic and potential interactions (both intra/intermolecular ones), are used to conform two memory functions of the system. Collective transport coefficients, such as shear and bulk viscosity, are calculated from these functions and their behaviour was systematically investigated as a function of flexibility and temperature.² It was found that including harmonic intramolecular stretching and bending terms (SPC/Fw³) the obtained viscosity values are in overall much better agreement than that of the rigid SPC/E model,⁴ compared to earlier and recent experimental data available.⁵ (See Figure 1).



The enhancement of concordance between data and the results coming from flexible model is patent in both shear and bulk viscosities. Nevertheless as temperature is lowered the agreement diverges implying an underlying many body interaction not entirely described in phenomenological approaches for intermolecular potentials. The effect of the intramolecular degrees of freedom on transport properties of liquid water was analyzed and incorporation of polarizability was discussed for further improvements.^{6,7} To our knowledge the present study constitutes the first such compendium of results for pure liquid water that has

been assembled.⁸

Figure 1: Shear Viscosity vs. Temperature. Rhomboes: SPC/E model. Triangles: SPC/Fw model. Star: Flexible Anharmonic Model. Circles: Experimental Data.⁵

¹ Evans D. J., Morriss G. P., *Statistical Mechanics of Nonequilibrium Fluids*, Anu E Press (2007),

² Medina J. S., *et al.*, *Inter. J. Quant. Chem.*, in press (2010),

³ Wu Y., *et al.*, *J. Chem. Phys.* **124**, 024503 (2006),

⁴ Berendsen H. J. C., *et al.*, *J. Phys. Chem.* **91**, 6269 (1987),

⁵ Korson L., *et al.*, *J. Phys. Chem.*, (1969), **73**, 34; Dukhin A. S., Goetz P. J., *J. Chem. Phys.* **130**, 124519 (2009),

⁶ Bukowski R., *et al.*, *J. Chem. Phys.* **128**, 094314 (2008),

⁷ Fanourgakis G. S., Xantheas S. S., *J. Phys. Chem. A* **110**, 4100-4106 (2006),

⁸ Medina J. S., *et al.*, *J. Chem. Phys.*, submitted (2010).

Attosecond XUV-IR laser pump-probe spectroscopy in H₂/D₂.

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The use of amplified femtosecond laser with a controlled carrier-envelope phase (CEP) has led to the generation of isolated attosecond laser pulses with durations as short as 80 as [1]. Attosecond pulses have been already used to control electron localization in D₂⁺ [2]. In this communication we have used attosecond pulses to excite and ionize H₂ molecules, which are subsequently probed in the attosecond time scale with a femtosecond (fs) pulse.

In the experiment an isolated XUV pulse of ~400 attosecond (as) with a low intensity (10⁹ W/cm²), produced through HHG in Krypton by means of a gating technique promptly photoionizes the D₂ (or H₂) molecule. Due to the wide photon energy spectrum (20-40 eV) associated to the as pulse, a large manifold of continuum as well as autoionizing states are populated. Several interfering pathways are then possible, direct dissociative and non dissociative ionization as well as autoionization from the Q_n doubly excited states. The molecule is then exposed to a moderately strong IR fs laser pulse (3x10¹² W/cm²) with a controlled time delay τ between the XUV and the IR pulse. D⁺ kinetic energy distributions collected within 45° along the polarization axis (mostly from parallel-oriented molecules) are measured as a function of time delay τ . Since the experiment may discriminate between D⁺ ions ejected in the upward (N_u) and the downward (N_d) directions along the molecular axis, we evaluate and plot the asymmetry parameter ($\beta=(N_u-N_d)/(N_u+N_d)$) as a function of the kinetic energy and the time delay. At long time delays $\tau > 10$ fs, the β parameter exhibits pronounced oscillations, which are the signature of electron localization during the molecular dissociation process. In contrast, at short time delays, the oscillations vanish progressively, which is the fingerprint of autoionization from the H₂ doubly excited states. This autoionization occurs within 1-5 fs after the XUV pump. For long time delays, the observations can be understood by solving the time dependent Schrödinger equation (TDSE) in a basis of two H₂⁺ molecular states [3]. To understand the observations for short time delays, we must include all electronic and vibrational degrees of freedom and to account for electron correlation. This is done by expanding the time dependent wave function in a large basis of H₂ vibronic states (typically > 100.000 states).

[1] Goulielmakis E *et al.* 2008 *Science* **320**, 1614

[2] Kling M F *et al.* 2006 *Science* **312**, 246

[3] Dietrich P *et al.* 1996 *Phys. Rev. Lett.* **77**, 4150

High-accurate potential surfaces and dynamics for He-I₂

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Ab initio CCSD(T) and MRCI approaches were employed to construct potential energy surfaces of the ground and the B electronic excited states of HeI₂ complex^{1,2}. For a direct comparison with the experiment, theoretical, accurate global PESs for both electronic states involved are required together with nuclear dynamics simulations.

Here, we present such fully quantum computation of the HeI₂ dynamics using the calculated surfaces. This allows us to make a first comparison with experiment based on first principles model potentials.

Binding energies, vibrationally averaged structures for both electronic states are determined, and their values are found to be in excellent accord with recent experimental measurements³. Further, spectral blueshifts and vibrational predissociation lifetimes are also computed and their comparison with the experimental data, in order to evaluate the quality of the *ab initio* surfaces, is discussed².

Such accurate model interaction potentials continue to be in demand for studying collisions of molecules with ultracold rare-gas atoms in optical traps, as well as spectroscopy of larger rare gas-dihalogen clusters, where a diatomic molecule interacts with a solvent system of rare gas atoms.

¹ R. Prosmi^{ti}, *et al.* *J. Phys. Chem. A*, **108**, 6065 (2004); L. García-Gutierrez *et al.* **113**, 5754 (2009).

² A. Valdés *et al.* *J. Chem. Phys.* **126**, 204301 (2007); **126**, 244314 (2007).

³ S. E. Ray, *et al.*, *J. Chem. Phys.*, **125**, 164314 (2006).

Eley–Rideal recombination of nitrogen on Tungsten(100)

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Among the different processes taking place at the gas-surface interface, molecular recombinations play a decisive role. The study and understanding of such mechanisms are a fundamental goal in surface chemistry.

Using the Classical Trajectory method, the dynamics of molecular recombination of nitrogen (N_2) from a Tungsten (W/100) surface is investigated, focusing our attention on the Eley - Rideal mechanism. The potential energy surface is an extended version of a periodic classical LEPS, recently developed in the group. Energy exchange between the nitrogen atoms and the surface as well as the solid temperature are accounted for using the Generalized Langevin Oscillator (GLO) model.

The Eley-Rideal dynamics is rationalized over a wide range of collision energies (0-3eV).

Dynamical study of the $O(^1D) + H_2(v_i=0, j_i=0) \rightarrow OH(X^2\Pi, v_f, j_f) + H$ reaction using the Mean Potential Phase Space Theory.

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State-to-state differential and integral cross sections for the title reaction have been calculated using the Mean Potential Phase Space Theory (MPPST) [1] on the ab initio ground $H_2O(X^1A')$ electronic state potential energy surface of Dobbyn and Knowles [2]. The integral and differential cross sections obtained are in excellent agreement with experimental measurements and with the benchmark predictions of the time-independent statistical quantum method and exact quantum mechanical wave packet method [3]. The calculated results confirm the dominance of the insertion mechanism and the relevance of using a simple statistical approach in describing complex-forming reaction dynamics. Additionally, proves the validity of the MPPST approach for the study of the title and similar indirect polyatomic reactions.

[1] P. Larrégaray, L. Bonnet, and J. C. Rayez, *J. Chem. Phys.*, 2007, **127**, 084308

[2] A. J. Dobbyn and P. J. Knowles, *J. Mol. Phys.*, 1997, **91**, 1107

[3] S. Y. Lin and H. Guo, *J. Chem. Phys.*, 2008, **129**, 124311

Quantum dynamics and ultrafast relaxation of photoexcited NO ($A^2\Sigma^+ \leftarrow X^2\Pi$) in cryogenic rare gas matrices

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Pump-probe techniques have proven to be a valuable tool for the study of the dynamics of excited states in the condensed phase, through the ultrafast detection of the dynamics of the optical and electronic properties of those systems. Within this context, many efforts have been addressed to the study of optical absorption in doped rare gas matrices. This technique offers the opportunity to obtain spectroscopic information on the host system and the impurity, since the excitation is usually localized on the latter, which acts as a chromophore. Among the wide variety of possible molecular targets, the lowest $A^2\Sigma^+$ Rydberg state of nitric oxide (NO) is amenable for femtosecond spectroscopy experiments [1,2]. The relaxation dynamics of NO doped neon matrices following the optical excitation of the molecular lowest Rydberg state has been the subject of previous pump-probe experiments [3-5]. After femtosecond excitation, an extensive lattice rearrangement occurs around the impurity. The latter is known as the formation of a microcavity or “electronic bubble”.

From the theoretical point of view, the theoretical description of these processes constitutes a remarkable challenge, due to the many-body character of this relaxation process and the presence of pronounced quantum effects. We present a detailed study of this process, both from a classical and quantum point of view:

- Molecular Dynamics (MD) simulations carried out on this system [4,6] incorporate the effect of zero point energy on the lattice atoms oscillations into MD simulations through an effective temperature derived within an harmonic approximation of crystal site oscillations [7] or its extension to anharmonic potentials [8]. Within this approach, the classical probability distribution at the effective temperature resembles the position dependence of the diagonal elements of the corresponding quantum density matrix. The influence of the effective temperature overestimation (within the quantum thermal harmonic correction) on the spectra and the relaxation dynamics of NO doped neon matrices has also been evaluated [9].
- A quantum shell model is presented, together with a direct solution of the multi-dimensional time-dependent Schrödinger equation. The model is based on a special parametrization of the potential energy surface, allowing to use the MCTDH method [10,11] for the high-dimensional quantum dynamics.

The excitation, bubble formation and subsequent vibrational relaxation is simulated, and compared to experimental results. The perspectives of this work include the extension to other quantum systems as well as other dynamical models, of both quantum and mixed quantum/classical nature

[1] L. Bonacina *et al.*, Phys. Rev. Lett. **95**, 015301 (2005)

[2] L. Bonacina *et al.*, J. Chem. Phys. **125**, 054507 (2006)

[3] M. Chergui *et al.*, J. Chem. Phys. **89**, 1277 (1988)

[4] F. Vigliotti *et al.*, Chem. Phys. Lett. **362**, 31 (2002)

[5] F. Vigliotti, L. Bonacina, and M. Chergui, Phys. Rev. B **67**, 115118 (2003)

[6] G. Rojas-Lorenzo *et al.*, Phys. Rev. B **67**, 115119 (2003)

[7] J. P. Bergsma *et al.*, J. Phys. Chem. **88**, 612 (1984)

[8] L. Uranga-Piña *et al.*, Chem. Phys. Lett. **429**, 450 (2006)

[9] L. Uranga-Piña *et al.*, submitted to Phys. Chem. Chem. Phys.

[10] MCTDH original references, plus Meier + Manthe MCTDH

[11] MCTDH Physics reports

Long range interaction inclusion in the HeH₂⁺ potential energy surface.

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The prototypical proton transfer process,



and its isotopic variants involving HD⁺ and D₂⁺ have been well investigated both experimentally^{1,2} and theoretically²⁻⁸. Besides being a test case of methods for ion molecule reactions, the above process is also important from the astrophysical point of view⁹⁻¹⁰. In order to explain the collisional outcomes of this reaction in various molecular beam experiments under different conditions, an accurate potential energy surface (PESs) is required.

To obtain an accurate potential energy surface for the HeH₂⁺, in our group we have introduced a new method¹¹ (that we have used to improve the H₃⁺ PES) of embedding the long-range interaction terms in the functional form used to represent the Potential Energy Surface of HeH₂⁺. Applications to the He + H₂⁺ reaction are presented. For the ground electronic state of HeH₂⁺ we use the Diatomics in Molecules (DIM) approach as a starting point, because it describes correctly the channels of dissociation. Usually the long-range terms are included *a posteriori* by using a switching function. The most widely used damping functions are probably those of Tang and Toennies¹², later modified to be an incomplete gamma function¹³. We will analyze the possibility of introducing the long-range terms *a priori*, by including them in the DIM approach.

¹ T. Turner, O. Dutuit, Y. T. Lee *J. Chem. Phys.* **81**, 3475 (1984).

² X.N. Tang et al. *J. Chem. Phys.* **122**, 164301 (2005).

³ T. Joseph, N. Sathyamurthy, *J. Chem. Phys.* **86**, 704 (1987).

⁴ B. Lepetit, J.M. Launay, *J. Chem. Phys.* **95**, 5159 (1991).

⁵ A. Aguado, M. Paniagua, *J. Chem. Phys.* **96**, 1265 (1992).

⁶ V. Aquilanti et al., *Chem. Phys. Lett.* **318**, 619 (2000).

⁷ P. Palmieri et al., *Mol. Phys.* **98**, 1835 (2000).

⁸ A.K. Tiwari, A.N. Panda, N. Sathyamurthy, *J. Phys. Chem. A.* **110**, 389 (2006).

⁹ L. Peroncelli, G. Grossi, V. Aquilanti, *Mol. Phys.* **102**, 21 (2004).

¹⁰ A.N. Panda, S.C. Althorpe, *Chem. Phys. Lett.* **419**, 245 (2006).

¹¹ L. Velilla et al. *J. Chem. Phys.* **129**, 084307 (2008).

¹² K.T. Tang and J.P. Tonnies. *J. Chem. Phys.* **66**, 1496 (1977).

¹³ K.T. Tang and J.P. Tonnies. *J. Chem. Phys.* **80**, 3726 (1984).

H₂ reactivity on gold clusters

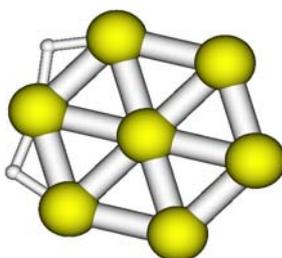
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Gold is the noblest of the transition metals and presents a very low reactivity in its bulk phase. However, in small gold nano-structures, the reaction barriers get lower and the chemisorption wells deeper for some reactions. Recently, this kind of systems have been studied with an increasing interest to determine their reactivity and their possible catalytic properties because their possible industrial impact¹. The dissociation of H₂ on nanowires and clusters^{2,3,4} have been studied, showing in some case small or no barrier and deep chemisorption wells for the dissociation reaction of H₂ on the clusters.

The reactivity is however no systematic in the different gold clusters and exhibits a high dependence on the geometry, the charge and the number of gold atoms in the cluster. The reasons of this dependences is not fully understood. In this work, we study the reactivity of H₂ on various Au_n (n=1-10) clusters which have been considered ionic or neutral. For a single gold atom, the reaction with H₂ is not favourable, however the metastable potential well of AuH₂, consequent to the stabilisation of excited p orbitales of the gold atom⁵ is suspected to be the precursor of the wells appearing in the bigger clusters. Furthermore of the potential wells, we study the reaction paths leading to them in the reactive cases. 2 kinds of mechanisms are observed, both leading to H atoms bounded to gold with double-bridge structure. The first involve 2 gold atoms, H₂ inserting itself between them before one of the two H jumps over one gold atom, like observed in linear chains⁶. The second involve only one gold atom which is directly attacked by the centre of H₂ bond, breaking it like a knife. This two mechanisms will be presented in details with the parameters which may favour them or not.



¹ A. Gorrane, A. Corma and H. García, *Science* 322 (2008)

² P. Jellinek, R. Pérez, J. Ortega and F. Flores, *Phys. Rev. Lett.* 96, 046803,(2006)

³ L. Barrio, P. Liu, J.A. Rodriguez, J. M. Campos-Martin and J.L.G. Fierro, *J. Chem. Phys.* 125, 124703 (2006)

⁴ A. Corma, M. Boronat, S. González and F. Illas, *Chem. Commun.*, 372 (2007)

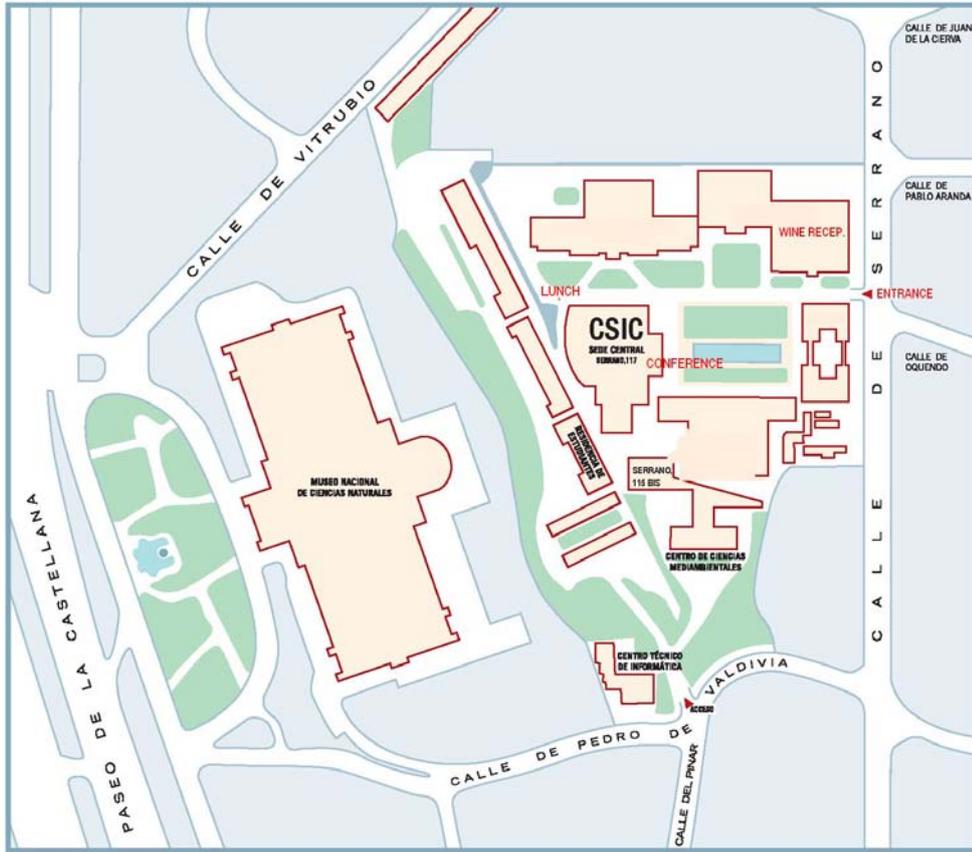
⁵ A. Zanchet, O. Roncero, S. Omar, M. Paniagua and A. Aguado, *J. Chem. Phys.* 132, 034301 (2010)

⁶ A. Zanchet, A. Dorta-Urra, O. Roncero, F. Flores, C. Tablero, M. Paniagua and A. Aguado, *Chem. Phys. Phys. Chem.* 11, 10122 (2009)

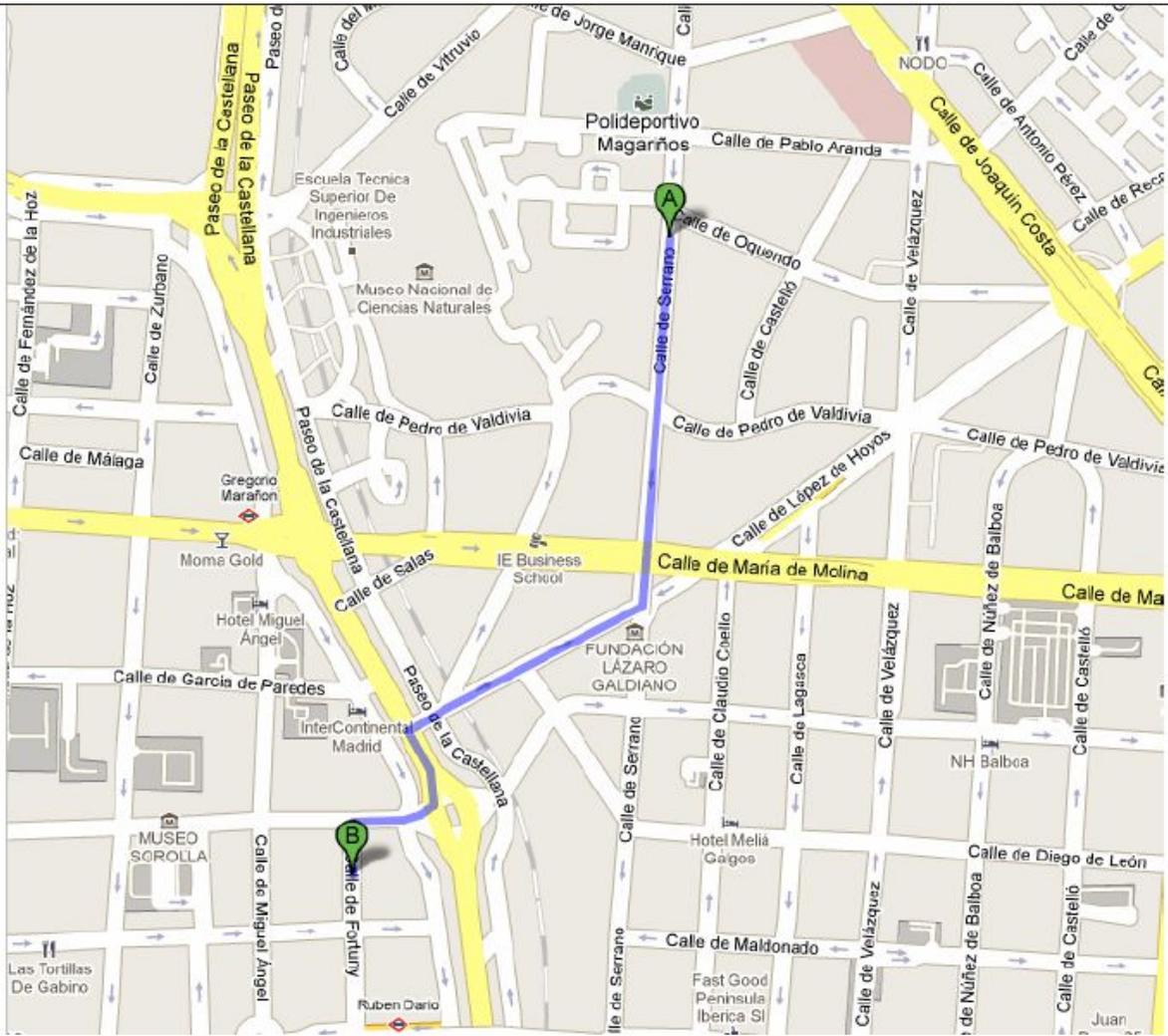
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Location of CSIC



Conference dinner

