Royal Society of Chemistry
Theoretical Chemistry Group

Newsletter − March 2003

Graduate Student Meeting − King's College, London
March 12th, 2003

The annual Theoretical Chemistry Group graduate student meeting will be held in Room 1.71, on the first floor of the Franklin−Wilkins Building, Stamford Street, London SE1 − on the Waterloo Campus of King's College London − on Wednesday March 12th from 13:30 to 17:30. This building is on the south side of the Thames, across Waterloo bridge from the Strand. The nearest tube station is Waterloo. A map can be found at http://www.kcl.ac.uk/maps/waterloo.html. The programme will consist of short talks presented by final year postgraduate students.

PROGRAMME

13:30	Prof. R. M. Lynden−Bell	Introduction
13:35	Mark Watson (Cambridge)	*Linear scaling of molecular Coulomb interactions by multipole expansions*
14:00	Iryna Rozum (UCL)	*Electron collisions with CF_x radicals*
14:25	Roma E. Oakes (Belfast)	*Interpreting Raman spectra using DFT methods*
14:50	Reimar Finken (Cambridge)	*Onsager model for a variable dielectric permittivity near an interface*
15:15	TEA	
15:45	Ahlam El−Barbary (Sussex)	*Ab initio calculations of point defects in graphite: structure,energetics and spectroscopy*
16:10	Thomas V. Mortimer−Jones (Birmingham)	*Ant Colony Optimization and its application to the protein folding problem*
16:35	Ross C. Walker (Imperial)	*"Lights, computer, action" − probing protein dynamics with QM/MM techniques and femtosecond laser spectroscopy*
17:00	M. Paul Gleeson (Manchester)	*Are QM/MM calculations useful in drug discovery?*
17:30	CLOSE	

All are welcome. There are no registration formalities.

Abstracts

Mark Watson (Cambridge)

Linear scaling of molecular Coulomb interactions by multipole expansions

We discuss the theory, implementation and application of multipole expansion methods in a Gaussian basis to treat the molecular Coulomb interaction with sub−quadratic cost using the electronic structure package Dalton.

Iryna Rozum (University College London)

Electron collisions with CF_x radicals

The purpose of this work is to develop a full description of electron CF_x radical collisions at energies up to 10 eV with particular emphasis placed on the energy range 2−5 eV as this is the typical energies of etching plasmas. We have performed calculations to obtain resonance parameters as well as elastic cross−sections and excitation cross−sections for the CF_2 and CF molecular radicals in the incident electron energy range below 10 eV. Several low lying resonaces were detected and fitted. We also performed several test target calculations for CF_3 for several target models using different basis sets (6−31G*, 6−311G* and Sadlej−pVTZ). Surprisingly, there are no data on vertical excitation energies of CF_3 available in the literature, so this is a necessary precursor to scattering calculations.

Roma E. Oakes (Queen's University, Belfast)

Interpreting Raman spectra using DFT methods

Density functional theory has been used to simulate and interpret the Raman spectra of fatty acid methyl esters − FAMEs (general formula $CH_3(CH_2)_nCOOCH_3$). We show that DFT enables secure vibrational mode assignments to be made, even in the case of complex Raman spectra and that the interpretation of the vibrational data can lead to a greater understanding of the experimental observations. Even very subtle effects seen in the experimental spectra have been reproduced in the calculated data. In addition, the correlations that allow the determination of chain−length and degree of unsaturation from inspection of Raman spectra have successfully been reproduced using DFT and the underlying physical reasons for their existence have been determined.

Reimar Finken (Cambridge)

Onsager model for a variable dielectric permittivity near an interface

Using a generalisation of an Onsager type approach, we are able to predict a dielectric permittivity profile of an inhomogeneous dipolar fluid in the presence of a dielectric interface. The reaction and cavity fields are calculated semi−analytically using bispherical coordinates. An asymptotic expression for the local permittivity is derived as a function of distance from the interface.

Ahlam El−Barbary (Sussex)

Ab initio calculations of point defects in graphite: structure, energetics and spectroscopy

We determine the structure and energetics of the point defects in graphite from first principles calculations. Particularly, we highlight the previously unreported behaviour that is a consequence of the symmetry−breaking Jahn−Teller distortion of the vacancy in graphite. Also, we explain the discrepancy between the experimental and the theoretical value for the migration energy. We comment on a major Wigner energy release which is found to be associated with the break up and recombination of an intimate or un−separated Frenkel pair. For the first time, we interpret the three−fold symmetry of the STM image of the vacancy in graphite as a three−fold thermally average, activated by a barrier of 0.13 eV. *Ab initio* EELS spectra for the topographical defects in graphite are obtained.

Thomas V. Mortimer−Jones (Birmingham)

Ant Colony Optimization and its application to the protein folding problem

Determination of the native state of a protein from its amino acid sequence is an important goal of protein folding simulations. Location of the global minimum structure (lowest energy folding conformation), however, is a difficult optimization problem. In this talk, we introduce Ant Colony Optimization, which is a recently developed method for global optimization, based on the behaviour of real ant colonies, and describe its application to study protein folding for the coarse−grained 2−D HP lattice bead model.

Ross C. Walker (Imperial College)

"Lights, computer, action" − probing protein dynamics with QM/MM techniques and femtosecond laser spectroscopy

The dynamics and flexibility of a protein are of fundamental importance in understanding the relationship between its structure and function. By applying linear response theory coupled to CIS calculations on molecular dynamics trajectories it has been possible to recreate the reorganisation energies and UV/VIS spectral widths of LADH and Zinc−myoglobin to within 10% of experiment. The method is sensitive enough to validate molecular dynamics force fields for chromophores and ultimately to allow the calculation of free energies of reactions for protein based systems.

M. Paul Gleeson (Manchester)

Are QM/MM calculations useful in drug discovery?

Methods based upon empirical force fields are the traditional way of studying small molecule−protein interactions relevant to drug discovery. We here show that in a number of cases, drug potency depends upon the formation of a covalent intermediate, and a situation arises where the use of the QM/MM method can lead to a quantitative understanding of the relationship between drug structure and activity.

Forthcoming Meeting

Modelling of Materials: Atomistic and Ab Initio Approaches

Mansfield College, Oxford (9−10 April 2003)

The Theoretical Chemistry Group and CCP5 are co−organising the above meeting, running from 2 p.m. on 9 April until 6 p.m. on 10 April. The meeting, which will be concerned with developments in methodology and algorithms for atomistic and ab initio simulations, as well as their applications, will consist of several invited lectures and a larger number of contributed talks, as well as a poster session.

Invited Speakers:
Neil Allan (Bristol), Emilio Artacho (Cambridge), Christian Elsaesser (Freiburg), Steve Parker (Bath), David Pettifor (Oxford), Joost VandeVondele (Cambridge), Mark Wilson (UCL).

Organizing Committee:
Ali Alavi (Cambridge), Saiful Islam (Surrey), Roy Johnston (Birmingham) .

Funding is gratefuly acknowledged from the Angela and Tony Fish bequest.

Please note: the lecture programme is now full, but participants and poster presentations are still welcomed. The registration deadline has been extended to **14 March 2003**.

For further details and to register see: http://www.tc.bham.ac.uk/~roy/TCG/Materials.html

Other Meetings of Interest

Faraday Discussion No. 124: *Quantum Inorganic Chemistry*

University of York, 14−16 April, 2003.

Details from Ms Christine Hall, Conference Department, Royal Society of Chemistry, Burlington House, Piccadilly, London W1J 0BA.

Web page: http://www.rsc.org/lap/confs/fara124.htm

Molecular and Solid State Quantum Chemistry

CLRC Daresbury Laboratory, 9 −10 June, 2003.

A meeting in honour of Vic Saunders.

Web page: http://www.cse.clrc.ac.uk/events/mssqc/index.htm

A Computational Approach to Chemistry

University of Warwick, 25 September, 2003.

A one day symposium to mark the retirement of David Hirst.

For more details see: http://www.tc.bham.ac.uk/~roy/TCG/hirst_meeting.txt

Report on previous meeting

Theoretical Chemistry Days No. 10

A half−day symposium on *The Application of Theory to Chemical Reactions at Surfaces* was held on Wednesday, 4th December, 2002 at University College, London. The introductory lecture was given by Professor Gerhard Ertl (Fritz Haber Institute, Berlin) with supporting lectures from Professors Richard Catlow (Royal Institution and University College, London) and David Bird (Bath) and Drs Peijun Hu (Belfast) and Ali Alavi (Cambridge). The meeting gave an excellent overview of theoretical methods (as well as experiments) which are being applied to study the physical properties of surfaces and the dynamics of reactions occurring on surfaces, including reactions of importance to heterogeneous catalysis. The meeting was well attended and the lectures stimulated lively discussion.

Positions Available

Computational Prediction of the Organic Solid State

Two computational postdoctoral positions and two PhD studentships
University College London / Royal Institution

As part of a major 4 year project on "Control and Prediction of the Organic Solid State" funded by the Basic Technology program, we are seeking research workers to develop computational methods of predicting organic crystal structures and polymorphism. The theoretical and computational developments will be performed in collaboration with experimental studies. Further details of the project and the individual positions are on http://www.chem.ucl.ac.uk/basictechorg/

The computational positions will be based in the Department of Chemistry at University College London and the closely connected Royal Institution, which are in central London. Candidates for the PDRA positions should have a PhD in atomistic computational chemistry using a variety of computational packages and computer systems, and preferably some familiarity with the organic solid state or nucleation processes. The gross annual salary, inclusive of London Weighting, will be approximately £26,000 for a four year contract for a recent doctoral graduate (point 6). The three year PhD studentships are funded as EPSRC project studentships, and therefore fully funded for maintenance and European Union fees. Please send a CV and contact details of two referees to Prof. Sally L. Price (s.l.price@ucl.ac.uk), who is happy to answer any further queries, before 28th April 2003.

Group Matters

Committee

The Group committee currently consists of Professor Ruth Lynden−Bell (Chairman − Belfast), Dr Roy Johnston (Secretary & Treasurer − Birmingham), Dr Ali Alavi (Cambridge), Dr Mike Bearpark (King's College, London), Dr Fred Manby (Bristol) and Professor Ian Williams (Bath).

Committee Vacancy

From January 2004, there will be a vacancy on the TCG committee. If you would like to volunteer or to nominate someone for this position (please check with the potential nominee first) please contact the Secretary at roy@tc.bham.ac.uk by **11 April**.

Membership

RSC members can join the Theoretical Chemistry Group by ticking the appropriate box on the RSC subscription form and paying the annual fee of £4. If you are an RSC member and wish to join part way through the year or if you are not a member of the RSC, please contact the RSC Membership Department. (For details see http://www.rsc.org/members/memindex.htm)

The Group web page (maintained by the RSC) is at http://www.rsc.org/lap/rsccom/dab/fara015.htm. More details about the Group, forthcoming meetings, etc. can also be found on http://www.tc.bham.ac.uk/~roy/TCG/TCG.html

If you are a member of the Group but are not on the e−mailing list, or if your e−mail address has recently changed, please contact the Secretary.

Newsletters

Please send material for inclusion in future newsletters (and for e−mail circulation and advertisement on the Group web site) to the Secretary, Dr R. L. Johnston, School of Chemical Sciences, University of Birmingham, Edgbaston, Birmingham B15 2TT (e−mail: roy@tc.bham.ac.uk).

TCG Annual Report and Accounts 2002

The annual report and accounts of the Group for 2002 will shortly be posted on the RSC web page at: http://www.rsc.org/lap/rsccom/dab/fara015.htm.

RSC Group Alerts

The RSC is introducing a "Group Alerts" e−mail scheme whereby group−related messages can be passed on to members of various special interest groups. You can register online at: http://www.rsc.org/CFReg/