Royal Society of Chemistry
Theoretical Chemistry Group

Newsletter − March 2002

Graduate Student Meeting − King's College, London
March 13th, 2002

The annual Theoretical Chemistry Group graduate student meeting will be held in Room 1B22 (First Basement, Strand Building), King's College, London on Wednesday March 13th from 13:30 to 17:45. The programme will consist of short talks presented by final year postgraduate students.

PROGRAMME

13:30	Prof. Ruth M. Lynden−Bell	*Introduction*
13:35	Martin J. Paterson (KCL)	*Conical intersections and inorganic photochemistry*
14:00	David Tew (Cambridge)	*Ro−vibrational calculations on molecules with wide amplitude motion: the reaction surface Hamiltonian*
14:25	Loredana Valenzano (Southampton)	*Nonadiabatic properties of the hydrogen molecular cation*
14:50	John P. Cole (Bristol)	*J conserving variational RRKM theory: application to branching ratios, product state and velocity distributions in time of flight photofragmentation spectra*
15:15		TEA
15:40	David Barker (Cambridge)	*Frozen density electron gas models of liquid water*
16:05	Thomas F. Miller III (UCL)	*Torsional path integral Monte Carlo method for the quantum simulation of biomolecules*
16:30	Gary Tresadern (Manchester)	*Modelling hydrogen tunnelling in enzymes*
16:55	Stephen Stackhouse (QMW)	*Ab initio studies of the clay mineral montmorillonite*
17:20	Graeme M. Day (UCL)	*Can vibrational, mechanical, and morphological calculations aid in polymorph prediction?*
17:45		CLOSE

All are welcome. There are no registration formalities.

Abstracts

Martin J. Paterson (KCL)

Conical intersections and inorganic photochemistry

Important conical intersections in two inorganic systems will be discussed. In the first study, it is shown, using a model chromophore−metal oxide complex, that a conical intersection is responsible for the ultrafast intermolecular charge injection between a squaraine dye and a wide band gap semiconductor (TiO_2). In the second study, the dynamics of $Cr(CO)_6$ photodissociation are studied using trajectory surface hopping methods to include non−adiabatic coupling. The decay of the $Cr(CO)_5$ photoproduct occurs through a Jahn−Teller type conical intersection which leads to the experimentally observed vibrational coherence.

David Tew (Cambridge)

Ro−vibrational calculations on molecules with wide amplitude motion: the reaction surface Hamiltonian

Since the Hamiltonian for the ro−vibrational motion in terms of internal coordinates becomes too complex as the size of the molecule increases, we return to normal coordinates. In terms of normal coordinates the description of wide amplitude motion, in particular internal rotation, becomes problematic. Previously the reaction path Hamiltonian has been employed to treat molecules with one wide amplitude motion. Here the reaction surface Hamiltonian is derived, allowing molecules with up to two wide amplitude motions to be treated. Ro−vibrational calculations on glyoxal using the reaction surface Hamiltonian are presented.

Loredana Valenzano (Southampton)

Nonadiabatic properties of the hydrogen molecular cation

A transformed hamiltonian theory combined with a scattering method is used to study nonadiabatic properties of vibration−rotation levels of the ground electronic states of H_2^+, D_2^+ and HD^+. The properties include bond length, dissociation energy and electric dipole polarizability. Progress towards the study of further properties will be reported.

John P. Cole (Bristol)

J conserving variational RRKM theory: application to branching ratios, product state and velocity distributions in time of flight photofragmentation spectra

Quantum phase space methods have been used in conjunction with total angular momentum conserving, variational Rice−Ramsperger−Kassel−Marcus (RRKM) theory to develop a new method for predicting the outcomes in a time of flight photofragmentation experiment. The methods will be described and will be compared with experiments for the photodissociation of ketene into two different sets of products.

David Barker (Cambridge)

Frozen density electron gas models of liquid water

A Kim−Gordon model has been developed for liquid water consisting of fixed molecular charge densities attached to molecular frames and coupled by a Thomas−Fermi−Dirac density functional hamiltonian (+ gradient corrections). This model has been implemented in a classical molecular dynamics code (DLPOLY) and successfully tested for liquid water. The purpose of the model is embedding of subsystems treated fully selfconsistently by orbital−based density functional methods. First results of this approach implemented in a Car−Parrinello code will also be discussed.

Thomas F. Miller III (UCL)

Torsional path integral Monte Carlo method for the quantum simulation of biomolecules

A molecular application is introduced for calculating quantum statistical mechanical expectation values of large molecules at non−zero temperatures. The Torsional Path Integral Monte Carlo technique applies an uncoupled winding number formalism to the torsional degrees of freedom in molecular systems. The internal energy of the molecules ethane, n−butane, n−octane, and enkephalin are calculated at standard temperature using the new technique.

Gary Tresadern (Manchester)

Modelling hydrogen tunnelling in enzymes

Hydrogen transfer, both protonic and hydridic, frequently contributes to the mechanism of enzyme catalysed reactions and is often rate limiting. Evidence for the importance of tunnelling in such reactions is found from the measured hydrogen kinetic isotope effects (KIE). We have used variational transition state theory (VTST) with multidimensional tunnelling corrections within a hybrid QM/MM formalism to understand the relationship between the potential energy surface and the measured KIE, which is central to relating enzyme structure to function.

Stephen Stackhouse (QMW)

Ab initio studies of the clay mineral montmorillonite

We present the results of density functional theory based calculations exploring the properties and behaviour of the clay mineral montmorillonite. In the first instance we explore the catalytic behaviour of sodium montmorillonite. This is in view of the recent discovery of the polymerisation of small organic molecules in the presence of the clay leading to favourable nanocomposite materials. Secondly we look at the effect of heating lithium montmorillonite, investigating such things as dehydroxylation and migration of small interlayer cations into the lattice structure.

Graeme M. Day (UCL)

Can vibrational, mechanical, and morphological calculations aid in polymorph prediction?

Computational searches for polymorphs have, until recently, involved locating minima in the lattice energy. Normally, a search generates far more energetically feasible structures than are known, so we are exploring the usefulness of other crystal properties in evaluating hypothetical structures. Lattice dynamical calculations have been performed to evaluate elastic constants and phonon frequencies. Such properties can highlight crystal instabilities and allow free energies to be compared. Furthermore, attachment energy calculations have been used to judge relative growth rates and evaluate structures on kinetic grounds.

Forthcoming Meeting

Exploring Modern Computational Chemistry (EMC2)

University of Nottingham, UK. 31 July−2 August, 2002.

An official satellite meeting of WATOC'02. Organised in association with the Theoretical Chemistry Group. Sponsored by Q−Chem Inc., Collaborative Computational Projects CCP5 and CCP6. Funding has also been received from the Angela and Tony Fish bequest of the Royal Society of Chemistry.

This international conference will bring together researchers in all aspects of modern computational chemistry. The programme will consist of invited lectures and a Poster session, which will be an integral part of the programme. Scientific Topics will include: Quantum Chemistry, Density Functional Theory, Structure and Spectroscopy, Intermolecular Potentials, Statistical Thermodynamics, Biological Applications.

Speakers who have accepted invitations include: A. Alavi (Cambridge), A. D. Becke (Queens', Ontario), C. R. A. Catlow (Royal Institution of Great Britain), D. C. Clary (University College London), J. N. L. Connor (Manchester), H. H. Fielding (King's College London), G. Frenking (Marburg), J. Gauss (Mainz), N. C. Handy (Cambridge), M. Head−Gordon (Berkeley), T. U. Helgaker (Oslo), I. H. Hillier (Manchester), K. N. Houk (UCLA) , W. M. Klopper (Utrecht), D. E. Logan (Oxford), R. M. Lynden−Bell (Queen's University Belfast), F. Manby (Bristol), A. B. McCoy (Ohio State), J. N. Murrell (Sussex), M. Orozco (Barcelona), J. A. Pople (Northwestern), S. L. Price (University College London), L. Radom (Australian National University), H. F. Schaefer III (Georgia), K. Szalewicz (Delaware), I. H. Williams (Bath), W. F. van Gunsteren (ETH).

Details from Dr J. D. Hirst, Department of Chemistry, University of Nottingham, University Park, Nottingham NG7 2RD, UK.

Web page (including pre−registration form): www.nottingham.ac.uk/chemistry/emc2.

Other Meetings of Interest

6th World Congress of Theoretically Oriented Chemists − WATOC'02
Lugano, Switzerland, 4−9 August, 2002.

Web page: http://www.watoc02.ch/

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

Report on previous meeting

Theoretical Chemistry Days No. 9

A half−day symposium on *Biological Applications of Electronic Structure Calculations* was held on Wednesday, 28th November, 2001 at University College, London. Lectures were given by Professors Per Siegbahn, Ian Hillier and Christopher Reynolds and Drs Adrian Mulholland and Jonathan Essex.

Positions Available

Lectureship in Computational/Theoretical Chemistry

Department of Chemistry and The Centre for Scientific Computing, University of Warwick.

See: http://www.warwick.ac.uk/jobs/job20104.html.

Applications in any field of Computational/Theoretical Chemistry are welcome for this joint appointment between the Department of Chemistry and the newly established University Centre for Scientific Computing.

The Centre for Scientific Computing involves researchers with interests in a variety of computational science disciplines, providing an opportunity to pursue interdisciplinary collaborations with biologists, computer scientists, mathematicians, and physicists. The Centre is concerned with improvement of algorithms, development of new computational methods, and exploitation of new developments in hardware and software technologies. The Department of Chemistry has a strong presence in theoretical and computational chemistry. The successful candidate will be expected to participate in teaching within the Department and to conduct research in both the Centre and the Department. Both the Department of Chemistry and the Centre for Scientific Computing have modern cluster computing resources, as well as visualisation hardware.

Further information may be obtained from Professor P J Derrick, Chair, Department of Chemistry, Professor Mike Allen, Director, Centre for Scientific Computing, or Professor Peter Taylor, Chief Scientist to the Centre for Scientific Computing. To apply, please see below.

Application forms and further particulars can be obtained from the Personnel Office, University of Warwick, Coventry CV4 7AL (telephone: 024 7652 3627) and from jobs.ac.uk/jobfiles/AC1372.html. Please quote reference 31/A/01. Closing date for applications is 28 March 2002.

Email: recruit@warwick.ac.uk

Postdoctoral Position

Department of Chemistry, University of Cambridge

Applicants are invited for a two year postdoctoral position with Professor Nicholas Handy, commencing 1st October, 2002, on aspects of Density Functional Theory.

Applications (c.v. and names of referees) should be submitted by post to: Professor Nicholas Handy, Department of Chemistry, Lensfield Road, Cambridge, CB2 1EW.

Group Matters

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

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).

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.

RSC members can join the Theoretical Chemistry Group by ticking the appropriate box on the RSC subscription form and paying the annual fee of £3. Others can join the Group by paying an annual fee of £7. 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.)

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.