Royal Society of Chemistry
Theoretical Chemistry Group

Newsletter - March 2004

Graduate Student Meeting - Imperial College, London
March 24th, 2004

The annual meeting for presentations by final year graduate students in theoretical chemistry will be held on the afternoon of Wednesday 24th March in Lecture Theatre C, RCS1 Building, Imperial College, London.

This year, the Group is introducing the Coulson Prize (in honour of the late Professor Charles Coulson) for the student who is judged to have presented the best talk at the meeting.

PROGRAMME

13:30	Prof. R. M. Lynden-Bell	*Introduction*
13:35	Darragh O'Neill (Nottingham)	*Hartree-Fock-Wigner Theory: a two-electron alternative to DFT*
14:00	Natalie Lambert (UCL)	*Computational and experimental studies of the bond-forming reactivity of multiply-charged cations with molecules in the gas phase*
14:25	Akyl Tulegenov (Nottingham)	*Alchemy with intermolecular potentials*
14:50	Oliver Lanning (Oxford)	*Screening at a charged surface by a molten salt*
15:15	TEA	
15:45	Ben Morgan (Oxford)	*Pressure driven transformations between tetrahedrally and octahedrally coordinated nanocrystals*
16:10	Tim Watson (Nottingham)	*Calculating vibrational frequencies of amides - from formamide to flavodoxin*
16:35	Dominic Clare (UCL)	*Molecular dynamics simulation of peptide-protein interactions*
17:00	Scott Habershon (Birmingham)	*Biologically-inspired computational chemistry: application to crystal structure determination from powder diffraction data*
17:30	Award Announcement and Presentation	
17:45	CLOSE	

All are welcome. There are no registration formalities.

Abstracts

Darragh O'Neill (Nottingham)

Hartree-Fock-Wigner Theory: a two-electron alternative to DFT

Hartree-Fock (HF) calculations account for approximately 99% of the total electronic energy in molecules. However, it is important to account for the final 1%, the electron correlation energy, for both qualitatively and quantitatively accurate results. Methods for treating electron correlation range from the computationally expensive wavefunction based methods (CI, CCSD, etc.) to the much cheaper density functional theories. We have recently introduced a method based on the Wigner intracule which gives a measure of the probability of finding two electrons at a point in phase space. In particular we use the HF intracule which results in a method which scales in an analogous way to HF calculations. We have parameterised our method using accurate calculations on the neon atom and this gives good estimates to the correlation energy of molecules. This can also be implemented in a self-consistent manner to allow geometry optimisation and frequency calculations.

Natalie Lambert (University College London)

Computational and experimental studies of the bond-forming reactivity of multiply-charged cations with molecules in the gas phase

Whilst the reactivity of multiply-charged ions is quite well understood in the context of aqueous media and metallic phases, relatively little is known of their chemical behaviour in the gas phase. It is only since the 1980's, due mostly to advances in experimental technology, that their role in the chemistry of extreme environments, such as the interstellar medium, planetary atmospheres and natural and man-made plasmas, has been revealed. In this talk I intend to present the results of our group's investigations into the bond-forming reactivity of a number of small atomic and molecular doubly-charged cations (dications) with molecules. These reactions are monitored experimentally by means of crossed-beam time-of-flight mass spectrometry. The potential energy surfaces of these reactions are then explored computationally in order to reveal the reaction mechanisms. Due to [dication + neutral] surfaces often existing as excited states of [monocation + monocation] surfaces, these calculations often require the use of sophisticated ab initio techniques such as CCSD(T) and QCISD(T). We have also found that for certain systems, the use of multireference methods such as MCSCF and MRCI are crucial in order to provide accurate descriptions of the potential energy surfaces.

Akyl Tulegenov (Nottingham)

Alchemy with intermolecular potentials

The SIMPER-P method to estimate intermolecular potentials for weakly bound systems is described. The potentials obtained using SIMPER-P are shown to be competitive in accuracy with those obtained from CCSD(T) ab-initio calculations. At the same time the computational expense is comparable to low-level methods (MP2). SIMPER-P is successfully tested on different systems (Ar-Ar, Ar-HF, Ar-H_2,H_2O-N_2).

Oliver Lanning (Oxford)

Screening at a charged surface by a molten salt

The screening of the electrical potential at a charged solid surface in a molten salt, KCl, has been investigated in a Molecular Dynamics simulation study. In the study the molten salt was confined between two rigid walls of equal and opposite charge. The relaxation time associated with the screening of the charged walls by the molten salt is found to be very short, and not dependent on diffusion. We also find that despite pronounced oscillatory structure in the charge density, the structure and dynamics of the ions close to the interface are very similar to those in the bulk.

Ben Morgan (Oxford)

Pressure driven transformations between tetrahedrally and octahedrally coordinated nanocrystals

The pressure-driven transformation of ionic nanocrystals, from the four coordinate zinc-blende to the six coordinate rocksalt crystal structures, have been studied using constant stress molecular dynamics, for system sizes ranging between 1000 and 4000 ions. A rigid-ion potential model was employed for the ion-ion interactions in the nanoparticles, and a binary Lennard-Jones system was used as a surrounding pressurising medium. Calculated diffraction patterns confirm the changes in the underlying crystalline structure, and the transformation mechanism is identified by following individual trajectories. This mechanism is found to be the same as has been observed in earlier simulations of bulk material, and provides a microscopic explanation for observed changes in the shape of the nanoparticle, and for the formation of grain boundaries, as well as the internal energy profile during the transformation.

Tim Watson (Nottingham)

Calculating vibrational frequencies of amides - from formamide to flavodoxin

The infrared (IR) is an information rich region of molecular spectra. From characteristic absorptions it is possible to determine much structural information about molecules. This has been used to a large degree in the study of protein structure as a complementary technique to circular dichroism, X-ray crystallography and NMR. However, the current understanding of protein IR spectra is predicated mainly on empirical structure-spectra relationships that are not infallible. Providing a theoretical basis for protein spectra will help to reduce these problems. This talk will outline the accurate methods used for small molecule calculations, their relationship to simpler methods for protein calculations and our current results.

Dominic Clare (University College London)

Molecular dynamics simulation of peptide-protein interactions

Protein-peptide interactions in aqueous solution have been probed using a molecular dynamics procedure with explicit solvent. An implicit solvent model has been used in post-processing with systematic mutation of each peptide residue to calculate binding free energies. Entropic contributions to the binding free energy have been estimated using classical ideal gas thermodynamics. The interaction between the oncoprotein Mdm2 and the tumour suppressor peptide p53 has been used as a test system. The method has been extended to study the interaction of IQN17, an HIV-1 gp41 mimic, with a potential fusion inhibitor D10-p1.

Scott Habershon (Birmingham)

Biologically-inspired computational chemistry: application to crystal structure determination from powder diffraction data

Many materials of interest, including pharmaceuticals, biomolecules, pigments and zeolites, cannot be easily prepared in the form of single crystals of sufficient size and quality for analysis by single-crystal diffraction techniques. In such cases, powder diffraction methods offer the only alternative route to complete structure determination. Consequently, recent years have witnessed an increasing interest in the development and application of new computational approaches aimed at aiding crystal structure determination from powder diffraction data. This presentation will highlight two recent aspects of work within this area. First, a new approach for determining unit cell parameters from powder diffraction data (commonly referred to as indexing) will be presented. Here, the indexing process is treated as a pattern recognition problem in which an Artificial Neural Network (ANN) is used to predict unit cell parameters from experimental powder diffraction data after analysis of the Bragg peak positions in powder diffraction patterns produced by known unit cells. Illustrative examples for orthorhombic systems will demonstrate the potential of this approach, and several aspects of the performance of the ANN will also be discussed. Secondly, recent developments of a Genetic Algorithm (GA) approach for direct-space crystal structure solution will be presented, with the focus being on improving the calculation speed and efficiency. Examples illustrating the current scope of this methodology will also be presented.

Forthcoming Meetings

The Theory of Chemical Dynamics
St. Edmund Hall, Oxford, 26-27 March 2004.

A symposium in honour of Professor Mark Child.
Web page: http://physchem.ox.ac.uk/~mano/markchild/

Bose-Einstein Condensation: From Atoms to Molecules
University of Durham, 30 March-3 April 2004.

Web page: http://www.dur.ac.uk/ccp6.workshop/2004/

Faraday Discussion No. 127: *Non-adiabatic Effects in Chemical Dynamics*
St Catherine's College, Oxford, 5-7th April 2004.

Web page: http://www.rsc.org/lap/confs/fara127.htm

Royal Society Discussion Meeting: *Configurational Energy Landscapes and Structural Transitions in Clusters, Fluids and Biomolecules*
The Royal Society, London, 19-20 April 2004.

Web page: http://www.chem.ucl.ac.uk/seminars/mcmrs/

RSC Faraday Division Symposium: *Computational Chemistry*
Geological Society Lecture Theatre, Burlington House, London, 29 April 2004.

Web page: http://www.rsc.org/pdf/faraday/fara290404.pdf

Symposium on Atomistic Simulation
Queen's University, Belfast, 21 May 2004.

A symposium in honour of Professor Ruth Lynden-Bell.
For details see: http://www.tc.bham.ac.uk/~roy/TCG/lynden-bell.txt

Molecular Quantum Mechanics: The No Nonsense Path to Progress
St John's College, Cambridge, 24-29 July 2004.

An international conference to honour the career of Professor Nicholas Handy.
Web page: http://www.ccc.uga.edu/Handy/

Report on previous meeting

Theoretical Chemistry Days No. 11

A half-day symposium (which was co-organised with CCP1) on *Excited States* was held on Wednesday 3rd December 2003 at University College, London. Plenary lectures were given by Professor Hans-Joachim Werner (University of Stuttgart) and Professor Hardy Gross (Free University, Berlin), with supporting lectures from Drs Nick Besley (Nottingham), David Tozer (Durham) and Tchavdar Todorov (Belfast). The speakers gave an excellent overview of *ab initio* electron correlation methods and time dependent density functional theory and their application to the study of excited states. The meeting was well attended and the lectures stimulated lively discussion. The Theoretical Chemistry Group is grateful to CCP1 for a significant contribution towards the speakers' travel expenses and to Professor Peter Knowles (chair of CCP1) for assistance in the organisation of the meeting.

Group Matters

Committee
The TCG Committee currently consists of Professor Ruth Lynden-Bell (Chair - Belfast), Dr Roy Johnston (Secretary & Treasurer - Birmingham), Dr Stuart Althorpe (Exeter), Dr Mike Bearpark (Imperial College, London), Professor Jonathan Hirst (Nottingham), Dr Fred Manby (Bristol), Dr David Tozer (Durham), Professor Ian Williams (Bath) and Dr Tim Wright (Sussex).

New Group Chairman
Professor Ruth Lynden-Bell's term of office is due to finish at the end of 2004. The new Chairman of the Group (who has been elected by the TCG Committee) is Professor Ian Williams, who will serve as Chairman for a period of 4 years, from January 2005.

Committee Vacancy

Due to Professor Williams' election as Chairman, there will be a vacancy for one person to serve on the TCG Committee for a period of 3 years, from January 2005. If you would like to volunteer or to nominate someone for this position (please check with the potential nominee first) please contact the Secretary (r.l.johnston@bham.ac.uk) by **30 April**. In the event of more than one person being nominated, an e-mail election will be held in May.

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). Please encourage your colleagues, postdocs and postgraduate students to join the Group.

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 at 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 (a number of e-mail addresses regularly fail), 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 Chemistry, University of Birmingham, Edgbaston, Birmingham B15 2TT (e-mail: r.l.johnston@bham.ac.uk).

Please note: by default, future newsletters will be sent out by e-mail (and mounted on the web site) only. If you wish to continue receiving a copy by regular mail, please notify the Secretary.

TCG Annual Report and Accounts 2003

The annual report and accounts of the Group for 2003 will shortly be posted on the RSC web page at: http://www.rsc.org/lap/rsccom/dab/fara015.htm.

RSC Group Alerts

You can register online at: http://www.rsc.org/CFReg.htm for the RSC's "Group Alerts" e-mail scheme, whereby group-related messages can be passed on to members of various special interest groups.