Royal Society of Chemistry
Theoretical Chemistry Group

Newsletter - November 2003

Theoretical Chemistry Days No. 11

Excited States

University College, London
December 3rd, 2003

The 2003 Theoretical Chemistry Day (which is being co-organised with CCP1) will be held in the Department of Chemistry, University College, Gordon Street at 1:30 p.m. on Wednesday, December 3rd.

PROGRAMME

13:30	Professor I. H. Williams	Introduction
13:35	Professor H.-J. Werner (Stuttgart)	*Ab initio calculation of excited states*
14:25	Dr N. A. Besley (Nottingham)	*A Wigner intracule based model of electron correlation in excited states*
15:00	TEA	
15:30	Professor E. K. U. Gross (Berlin)	*Time-dependent density functional theory: Moving from the linear to the non-linear domain*
16:20	Dr D. J. Tozer (Durham)	*Excitation energies in time-dependent density functional theory: The importance of the integer discontinuity*
16:55	Dr T. Todorov (Belfast)	*Power dissipation in atomic-scale conductors: Quantum, classical and mixed quantum-classical dynamics*
17:30	CLOSE	

All are welcome. There are no registration formalities.

Meetings Held During 2003

Graduate Student Meeting 2003

A meeting of the Theoretical Chemistry Group was held on 12th March, 2003 at King's College, London. Eight presentations were made by final year graduate students on a wide range of topics: linear scaling of molecular Coulomb interactions; theoretical studies of electron-radical collisions; interpreting Raman spectra using DFT calculations; studies of dielectric permittivity near an interface; *ab initio* calculations of defects in graphite; theoretical study of protein folding; and the application of QM/MM calculations to study protein dynamics and drug molecule design. The overall standard of the presentations continues to be very high.

Modelling of Materials: Atomistic and Ab Initio Approaches

Mansfield College and the Physical and Theoretical Chemistry Laboratory, Oxford (9-10 April 2003)

This meeting, which was co-organised with CCP5, was concerned with developments in methodology and algorithms for atomistic and *ab initio* simulations of materials, as well as their applications. It consisted of invited lectures from Neil Allan (Bristol), Emilio Artacho (Cambridge), Christian Elsaesser (Freiburg), Steve Parker (Bath), David Pettifor (Oxford), Joost VandeVondele and Mark Wilson (UCL), along with 18 contributed lectures and 19 contributed posters. The meeting was well attended (with a total of 56 registered delegates) and was felt to be timely, with the combination of delegates from different areas of materials modelling working particularly well.

Funding is gratefuly acknowledged from CCP5 and the Angela and Tony Fish bequest.

Future Meetings

Graduate Student Meeting 2004

The annual meeting for presentations by final year graduate students will be held in March 2004 (date and venue to be arranged). Offers of contributions (title and short abstract) should be sent to the Secretary by February 1st.

Other Forthcoming Meetings of Interest

The Theory of Chemical Dynamics

A Symposium in Honour of Professor Mark S. Child

St. Edmund Hall, Oxford (26-27 March 2004)

Organisers: D. C. Clary, P. J. Grout, D. E. Logan, P. A. Madden, D. E. Manolopoulos

Speakers: S. K. Gray (Argonne), L. Halonen (Helsinki), E. J. Heller (Harvard), C. Jungen (Paris-Sud), R. A. Marcus (Caltech), W. H. Miller (Berkeley), E. Pollak (Weizmann), J. N. Tennyson (UCL), T. Uzer (Georgia Tech.), K. B. Whaley (Berkeley).

Further details and registration: Please contact P. C. Dunn, Physical and Theoretical Chemistry Laboratory, South Parks Road, Oxford OX1 3QZ, U.K. (email: thchem@physchem.ox.ac.uk).

CCP6 Workshop 2004: *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 (5-7 April 2004).

For details contact: Christine Hall, Scientific Affairs and Conferences, Royal Society of Chemistry, Burlington House, Piccadilly, London W1J OBA, tel +44 (0) 20 7437 8656, fax +44 (0) 20 7734 1227, Email hallc@rsc.org

Any queries regarding scientific matters should be referred to: Professor Mark S Child, University of Oxford, Physical and Theoretical Chemistry Lab., South Parks Road, Oxford OX1 3QZ, UK, tel +44 (0) 1865 275 151, fax +44 (0) 1865 275 430, Email: mark.child@chemistry.oxford.ac.uk

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).

Organisers: Paul McMillan (UCL) and David Clary (Oxford). Registration is free and you can now register for the meeting at https://www.royalsoc.ac.uk/events/forms/apr04_form.htm.

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

Molecular Quantum Mechanics: The No-Nonsense Path to Progress

An international conference to honour the career of Professor Nicholas Handy

St John's College, Cambridge (24-29 July 2004).

Organisers: David Clary (Oxford), Sue Colwell (Cambridge), Fritz Schaefer (Georgia, USA).
It is now possible to register for this meeting.

Web page: http://zopyros.ccqc.uga.edu/Handy/

See the **Royal Society of Chemistry list of conferences and events** on the web at http://www.chemsoc.org/events/conhome.htm

The Second Industrial Fluid Properties Simulation Challenge

Scientists from 3M, BP, the Dow Chemical Company, DuPont, Mitsubishi Chemicals, and the National Institute of Standards and Technology (NIST) have announced the problems for the Second Industrial Fluid Properties Simulation Challenge. Academic groups, research laboratories, and scientific software companies from around the world have just over a year to predict vapor pressures and heats of vaporization, gas solubility, and enthalpies of mixing for materials specified by the contest committee. During the year accurate experimental measurements of these properties will be obtained by scientists at NIST and the Dow Chemical Company. These experimental data will be used to judge the predictions made by the contest entrants. Champions will be announced and prizes awarded at a special session at the AIChE National Meeting in November 2004.

For a full version of the announcement see: http://www.tc.bham.ac.uk/~roy/TCG/fluid.doc.

Contact: Fiona Case
Email: fiona@casescientific.com
Website: http://www.cstl.nist.gov/FluidSimulationChallenge/.

Vacancies

PhD Studentship in Theoretical Condensed Matter Chemical Physics

Department of Chemistry, Imperial College London

Applicants must be home students and must have at least a 2:1 Honours MSci or MChem degree or an MSc in Physics. The Stipend is £10,750 p.a.

For further details contact
Professor Alexei Kornyshev (http://www.ch.ic.ac.uk/kornyshev/),
Department of Chemistry, Imperial College London, London SW7 2AY
e-mail A.Kornyshev@imperial.ac.uk ;
tel: 020 7594 5786.

For an application form contact Doris Pappoe: d.pappoe@imperial.ac.uk or download the form from www.imperial.ac.uk/pgoptions.

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 Michael Bearpark (King's College, London), Dr Fred Manby (Bristol) and Professor Ian Williams (Bath). Ali Alavi's term on the committee finishes at the end of December 2003 and we wish to thank him for his activities on behalf of the Group over the past three years. From January 2004 the committee will be expanded, with four new members: Dr Stuart Althorpe (Exeter), Dr Jonathan Hirst (Nottingham), Dr David Tozer (Durham) and Dr Tim Wright (Sussex).

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 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, 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: roy@tc.bham.ac.uk).

TCG Annual Report and Accounts 2002

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

RSC Group Alerts

The RSC has introduced 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/.