

Royal Society of Chemistry Theoretical Chemistry Group

Newsletter - November 2004

Theoretical Chemistry Days No. 12

Controlling Atoms and Molecules: In Theory and Practice

University College, London
November 10th, 2004

The 2004 Theoretical Chemistry Day (which is being co-organised with the Chemical Physics group of the Institute of Physics) will be held in the Department of Chemistry, University College, Gordon Street on Wednesday, November 10th.

PROGRAMME

10.30 Coffee available

11.00 Prof. Ferenc Krausz (Vienna) *Attosecond Physics: Controlling and Tracking Electronic Dynamics*

11.45 Prof. Gabriel Balint-Kurti (Bristol) *Ab Initio Theory of Laser Pulse Design to Control Molecular Quantum States*

12.30 Lunch

2.00 Prof. Hershel Rabitz (Princeton) *Controlling Quantum Dynamics Phenomena With Photonic Reagents*

2.45 Dr Simon Hooker (Oxford) *Extreme Ultraviolet and Soft X-Ray Lasers*

3.30 Tea

3.50 Prof. Helen Fielding (UCL) *Optical Control of Electron Wave Packets*

4.35 Prof. Jeremy Hutson (Durham) *Ultracold Molecules and their Collisions*

5.20 Dr Stuart Althorpe (Exeter) *The Berry Phase and the Simplest Chemical Reaction*

6.05 END

For further details see: <http://groups.iop.org/CH/UCL.html>
<http://cadmium.chem.ucl.ac.uk/iop/>

All are welcome. There are no registration formalities.

Meetings Held During 2004

Graduate Student Meeting 2004

A meeting of the Theoretical Chemistry Group was held on 24th March, 2004 at Imperial College, London. Eight presentations were made by final year graduate students on a wide range of topics: Hartree-Fock-Wigner theory; studies of reactivity of multiply-charged ions; alchemy with intermolecular potentials; simulation of molten salts; pressure driven transformations in nanocrystals; calculating vibrational frequencies of amides; MD simulations of peptide-protein interactions; biologically-inspired computational chemistry. The overall standard of the presentations, as usual, was very high, which made the awarding of the Coulson prize (see below) a difficult task.

The Coulson Prize 2004

The recipient of the TCG's inaugural Coulson Prize for the student judged to have presented the best talk at the TCG Graduate Student Meeting, was Natalie Lambert of University College, London for her talk on computational and experimental studies of bond-forming reactivity of multiply charged cations with molecules in the gas phase. Natalie has been presented with a cheque and will receive a certificate.

Future Meetings

Graduate Student Meeting 2005

The annual meeting for presentations by final year graduate students will be held in March 2005 (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

11th International Conference on the Applications of DFT in Chemistry and Physics

Geneva, Switzerland, 11-15 September 2005.

For details see: <http://DFT2005.unige.ch>

Vacancies

Postdoctoral Fellowships at the Australian National University

Professor Peter Gill has two postdoctoral vacancies in his group at the Australian National University in Canberra.

Please see <http://rsc.anu.edu.au/employment.php> for details.

PhD & Postdoctoral Opportunities in Computational Chemistry & Bioinformatics

with Professor Jonathan Hirst, School of Chemistry, University of Nottingham. All posts are available from 1st April, 2005 onwards; UK and EU citizens are eligible for the studentships.

PhD studentship – computational studies of protein conformation and spectroscopy.

2 PhD studentships and one Postdoctoral Research Associate – bioinformatics studies of protein structure in collaboration with the School of Computer Science & IT, University of Nottingham.

To apply or for further details please email jonathan.hirst@nottingham.ac.uk.

1 Postdoctoral Research Associate and 1 PhD Studentship in Theoretical Chemistry

Department of Chemistry, Cambridge, UK.

Applications are invited for a postdoctoral research associate and a PhD student to work in the group of Dr David Wales on an EPSRC-funded project on the theory and computer simulation of protein folding dynamics.

Research Associate

Applicants for the post-doctoral position should have a PhD in a relevant area of chemical physics. Experience of large-scale biomolecular simulation would be particularly advantageous. The pensionable salary will be in the range £19,460 to £29,127 p.a., depending on experience. The post is available from January 2005 and appointment will be for three years, subject to a probation period of six months. Applications should include a full CV, publications list, and the names of two referees. They should be accompanied by a completed form PD18 (downloadable from <http://www.admin.cam.ac.uk/offices/personnel/forms/pd18>).

PhD studentship

Applicants for the PhD studentship should have or expect to receive a first class honours degree involving theoretical chemistry or physics. The studentship is available only to EU citizens who satisfy the residence requirements of the UK Research Councils. Applications should include a CV, and the names of two referees.

Applications for both vacancies should be sent to Dr David Wales, Department of Chemistry, Lensfield Road, Cambridge CB2 1EW (tel: 01223 336354; fax 01223 336362; email: dw34@cam.ac.uk).

Closing date: 30 November.

The University is committed to equality of opportunity.

Group Matters

The Group committee currently consists of Professor Ruth Lynden-Bell (Chairman - Cambridge), Dr Roy Johnston (Secretary & Treasurer - Birmingham), Dr Stuart Althorpe (Nottingham), Dr Michael Bearpark (Imperial College, London), Professor Jonathan Hirst (Nottingham), Dr Fred Manby (Bristol), Dr David Tozer (Durham), Professor Ian Williams (Bath) and Dr Tim Wright (Nottingham). Professor Lynden-Bell's term as Chairman of the committee finishes at the end of December 2004 and we wish to thank her for all of her activities on behalf of the Group in recent years. From January 2005, Ian Williams will be taking over as Chairman of the Group (for a period of 4 years) and the committee will have two new members: Dr Nik Kaltsoyannis (University College, London) and Dr John Wilkie (Birmingham), who will serve for 3 years.

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.

Group Web Page

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).

TCG Annual Report 2003

The annual report of the Group for 2003 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/>.