

## Theoretical Chemistry Group

Newsletter – November 2008

### *Theoretical Chemistry Day #16*

*Organized in association with the Molecular Graphics and Modelling Society*

### Computational Biospectroscopy

Wednesday 3 December

Imperial College London

Department of Chemistry, South Kensington Campus  
Registration is free and there are no registration formalities

13:45 Welcome

13:50 Jennifer Herek (University of Twente)

*Coherent control of complex molecules: from blind optimization to insight on mechanism*

14:30 David Klug (Imperial College London)

*The new world of Coherent Multidimensional Spectroscopy: Implications for the study of protein dynamics, structure, composition and function*

15:00 Laurence Barron (University of Glasgow)

*Solution Structures of Biomolecules from Experimental and Theoretical Raman Optical Activity Spectra*

15:30 Refreshment Break

16:00 Stephen Meech (University of East Anglia)

*Ultrafast Dynamics in Photoactive Proteins: Investigating the Role of Hydrogen Bonds and Proton Transfer*

16:30 Nick Besley (University of Nottingham)

*Quantum Chemical Calculations of the Spectroscopy of Metalloproteins*

17:00 Nikos Doltsinis (King's College London)

*Shedding light on (the) matter: ab initio simulations of photoactive materials*

17:30 Close

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## Forthcoming Meetings

**Computer Aided Molecular Design** at The Jolly Beach Resort, Bolans Village, Antigua and Barbuda, 18<sup>th</sup> March, 2009 – 21<sup>st</sup> March, 2009. For more details, please visit the website <http://www.zingconferences.com/z.cfm?c=61>



Speakers include:  
Andrew Good (*Bristol-Myers Squibb*)  
Andrew Leach (*GlaxoSmithKline*)  
Emily Carter (*Princeton*)  
Eugene Shakhnovich (*Harvard*)  
Jeffrey Skolnick (*Georgia Institute of Technology*)  
Richard Catlow (*UCL*)  
Tom Blundell (*Cambridge*)  
William Jorgensen (*Yale*)

The deadline for Earlybird registration (\$999) is the 18<sup>th</sup> December, 2008. RSC Theoretical Chemistry Group members can register at the super Earlybird rate of \$899 (\$625 students). Registration fees are all-inclusive of accommodation and meals.

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MGMS Young Modellers' Forum, The Brunei Gallery, School of Oriental & African Studies (SOAS), London, 28th November 2008. For more details, please visit the Young Modellers' Forum home page <http://www.mgms.org/YMF2008/YMF2008.html>

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CCPB third annual conference – “Biomolecular Simulation 2009”, Yorkshire Museum and Gardens in York, from Tuesday 6<sup>th</sup> till Thursday 8<sup>th</sup> January 2009. For more details, please visit: <http://www.ccpb.ac.uk/events/conference/2009/>

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13<sup>th</sup> International Congress on Quantum Chemistry, 22-27 June 2009, Helsinki, Finland  
<http://www.helsinki.fi/kemia/icqc>

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7<sup>th</sup> Canadian Computational Chemistry Conference, 20-24 July 2009, Halifax, Nova Scotia  
<http://www2.bri.nrc.ca/cccc7>

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4<sup>th</sup> Asian Pacific Conference on Theoretical and Computational Chemistry, Singapore, December 2009 (Richard Wong)

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Molecular Quantum Mechanics: from methylene to DNA and beyond - in honour of H. F. Schaefer, 24-29 May 2010, Berkeley, California (Rod Bartlett)

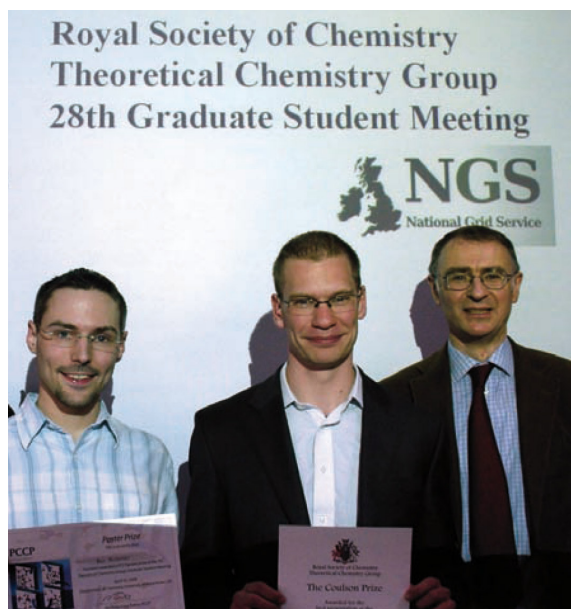
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9<sup>th</sup> WATOC, 17-22 July 2011, Santiago de Compostela, Spain  
(Manuel Yañez)

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## Report on Previous Meetings

The annual meeting for presentations by final year graduate students in theoretical chemistry was held on Wednesday 16<sup>th</sup> April, 2008, at the University of Manchester. The student talks were book-ended by contributions from more senior researchers. The meeting opened with a lecture from Professor Ian Hillier (Manchester) on “*Quantum Chemistry Calculations; Search for the last kilojoule or solve chemical problems?*” Then, Slimane Doudou (Manchester) spoke on “*Protein-ligand binding energetics and mechanisms*”, followed by Ben Bulheller (Nottingham) on “*Computing Dichroism of Proteins*”. A poster session was held over lunch. Talks after lunch were presented by Andrew Mitchell (Oxford) “*N Novel correlated states with coupled quantum dots*”, Lauro Oliver Paz-Borbon (Birmingham) on “*Theoretical studies of bimetallic clusters: 2row - 3row Transitions Metals*”, Shanthi Pandian (Manchester) on “*Enzymatic evolution: a single mutation to chlorinate or hydroxylate? A DFT study of a non-heme halogenase*”, and James Spencer (Cambridge) on “*Beyond Hartree-Fock: ab-initio approaches to correlation in periodic systems*”. The closing lecture was delivered by Dr Chris Skylaris (Southampton), who spoke about “*The ONETEP method for linear-scaling DFT calculations*”. A Poster Prize, kindly sponsored by *Phys Chem Chem Phys* was awarded to Ben Bulheller. The Coulson Prize for 2008 was awarded to Andrew Mitchell of the University of Oxford.



Prize winners, Andrew Mitchell (centre) and Ben Bulheller (left), and the Chair of the TCG, Ian Williams (right) at the Graduate Student meeting of the TCG.

## **Announcement**

The Royal Society of Chemistry is launching a book series in Theoretical Chemistry. If you have a proposal for a book, please contact the Series Editor: Jonathan Hirst (email: [jonathan.hirst@nottingham.ac.uk](mailto:jonathan.hirst@nottingham.ac.uk)).

## **Group Matters**

### **Committee**

The TCG Committee currently consists of Professor Ian Williams (Chair – Bath), Professor Jonathan Hirst (Secretary & Treasurer – Nottingham), Dr Tanja van Mourik (St Andrews), Dr Katherine Thompson (Birkbeck College), Dr Massimo Mella (Cardiff), Dr Paul Popelier (Manchester), Dr David Wales (Cambridge).

### **Group Web Page**

The Group web page (maintained by the RSC) is at <http://www.rsc.org/tcg>. If you have any items for inclusion on the web site, please contact the Secretary.

### **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 £5. 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/images/JoinaGroup\\_tcm18-107316.pdf](http://www.rsc.org/images/JoinaGroup_tcm18-107316.pdf)). Please encourage your colleagues, postdocs and postgraduate students to join the Group.

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: Professor Jonathan Hirst, School of Chemistry, University of Nottingham, University Park, Nottingham NG7 2RD (e-mail: [jonathan.hirst@nottingham.ac.uk](mailto:jonathan.hirst@nottingham.ac.uk)).