Starting salary on scale £18,265 − £20,311 a year depending on experience and qualifications; some financial assistance with relocation and mobility is also available. Each post is available immediately for a period of 12 months.

Informal enquiries to Dr. R. L. Johnston tel 0121 414 7477, roy@tc.bham.ac.uk, or Prof. Peter Knowles tel: 0121 414 7472, p.j.knowles@bham.ac.uk Application forms (returnable by 12th December 2002) and details from: Personnel Services, The University of Birmingham, Edgbaston, Birmingham, B15 2TT, U.K. Tel: +44−121 414 6486. Web: www.bham.ac.uk/personnel/

Postdoctoral Research Associate − *Electronic Excited States of Amides*

School of Chemistry, University of Nottingham

Applicants are invited to apply for an EPSRC funded postdoctoral position to work on electronic structure calculations on amides with Dr Jonathan Hirst. The project will involve using the latest quantum chemical methods, including time−dependent density functional theory, to characterise the electronic excited states of amides, with the aim of providing a better understanding of the electronic structure of proteins. Salary will be within the range £17,626 to £19,681 per annum, depending on qualifications and experience. The post is available from January, 2003. The appointment will be for one year, in the first instance. Candidates should have a PhD in the Physical Sciences. Programming experience and familiarity with quantum chemical methods is desirable.

Candidates should send a detailed CV, together with the names and addresses of two referees, to Dr J D Hirst, School of Chemistry, The University of Nottingham, University Park, Nottingham, NG7 2RD. Informal enquiries may be addressed to Dr Jonathan Hirst, Email: Jonathan.Hirst@Nottingham.ac.uk. Further details are also available on at: http://slater.chem.nott.ac.uk/~jhirst/Public/index.html.
Closing date: 6th December, 2002.

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).

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 £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.)

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.

RSC Group Alerts

The RSC is introducing a "Group Alerts" e−mail scheme whereby group−related messages can be passed on to members of various special interest groups. Please let me know if you wish me to pass on your e−mail address, or register online yourself at: www.rsc.org/CFReg/

Royal Society of Chemistry
Theoretical Chemistry Group

Newsletter − November 2002

Theoretical Chemistry Days No. 10
The Application of Theory to Chemical Reactions at Surfaces

University College, London
December 4th, 2002

The 2002 Theoretical Chemistry Day will be held in the Department of Chemistry, University College, Gordon Street at 1:30 p.m. on Wednesday, December 4th.

PROGRAMME

13:30	Prof. R. M. Lynden−Bell	*Introduction*
13:35	Prof. G. Ertl (Berlin)	*Dynamics of reactions at surfaces*
14:25	Prof. C. R. A. Catlow (RI & UCL)	*Modelling catalytic reactions on oxide surfaces*
15:10	TEA	
15:40	Prof. D. Bird (Bath)	*Electron−hole pair excitation in H/Cu(111) dynamics*
16:15	Dr P. Hu (Belfast)	*An understanding of reaction sites in heterogeneous catalysis*
16:50	Dr A. Alavi (Cambridge)	*Density Functional Theory simulation of metal surfaces*
17:30	CLOSE	

All are welcome. There are no registration formalities.

Meetings held during 2002

Graduate Student Meeting 2002

A meeting of the Theoretical Chemistry Group was held on 13th March, 2002 at King's College, London. Nine presentations were made by final year graduate students on a wide range of topics including: theoretical studies of photochemistry and spectroscopy; modelling liquid water and biomolecules; and applications of theory in solid state and structural chemistry. The overall standard of the presentations continues to be very high.

Exploring Modern Computational Chemistry (EMC2)

University of Nottingham, 31 July−2 August, 2002.
This was an official satellite meeting of WATOC'02 and was organised in association with the Theoretical Chemistry Group and the Statistical Mechanics and Thermodynamics Group. The meeting was well attended and had an excellent line up of speakers from the UK and overseas. The organisers are grateful for funding from a number of sources, including the Angela and Tony Fish bequest.

Future Meetings

Graduate Student Meeting 2003

The annual meeting for presentations by final year graduate students will be held on the afternoon of Wednesday 12th March 2003 at King's College, London. Offers of contributions should be sent to the Secretary by February 1st. Please send a title and a short abstract.

Modelling of Materials: Atomistic and Ab Initio Approaches

Mansfield College, Oxford (9−10 April 2003)

The Theoretical Chemistry Group and CCP5 are co−organising the above meeting, running from 2 p.m. on 9 April until 6 p.m. on 10 April. The meeting, which will be concerned with developments in methodology and algorithms for atomistic and ab initio simulations, as well as their applications, will consist of several invited lectures and a larger number of contributed talks. Offers of talks from postgraduate students and postdocs are particularly encouraged.

Invited Speakers:
Neil Allan (Bristol), Emilio Artacho (Cambridge), Christian Elsaesser (Freiburg), Steve Parker (Bath), David Pettifor (Oxford), Joost VandeVondele, Mark Wilson (UCL).

Organizing Committee:
Ali Alavi (Cambridge), Saiful Islam (Surrey), Roy Johnston (Birmingham) .

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

Please address any queries or offers of contributed talks to Roy Johnston (roy@tc.bham.ac.uk).
For further details and to register see: http://www.tc.bham.ac.uk/~roy/TCG/Materials.html

Registration Deadline: February 15th 2003.

Other Meetings of Interest

CCP1/CCP6/ChemReact Workshop

High Accuracy Potentials for Quantum Dynamics

University College, London, 31 March−2 April 2003.

Invited Speakers:
Wim Klopper (Utrecht), Attila Császár (Eötvös Loránd University), Kirk Peterson (Washington State University), Peter Taylor (Warwick), Hans−Joachim Werner (Stuttgart), Krzysztof Szalewicz (Delaware), Ad van der Avoird (Nijmegen), David Schwenke (Nasa Ames Research Center), Oleg Polyansky (UCL), Pavel Rosmus (Marne la Vallée), Colin Western (Bristol), Antonio Varandas (Coimbra), David Yarkony (Johns Hopkins University), Timothy Lee (Nasa Ames Research Center), Harry Quiney (Melbourne).

Scientific/Organizing Committee:
Jonathan Tennyson (UCL), Peter Knowles (Birmingham), Jeremy Hutson (Durham), Gabriel Balint−Kurti (Bristol), Andrea Miani (UCL), Tanja van Mourik (UCL).
For further information and to register, see: http://www.tampa.phys.ucl.ac.uk/workshop

Registration Deadline: February 1st 2003.

Faraday Discussion No. 124: *Quantum Inorganic Chemistry*

University of York, 14−16 April, 2003.

For details contact Dr Nik Kaltsoyannis (uccanka@ucl.ac.uk) or Penny Mohammed (mohammedp@rsc.org). Web page: http://www.rsc.org/lap/confs/fara124.htm

Positions Available

2 Postdoctoral Research Assistants in Theoretical Chemistry

School of Chemical Sciences, University of Birmingham

Applications are invited for two 12−month postdoctoral fellowships associated with the European Commission Research Training Network "*THEONET II: Theoretical studies of electronic and dynamical processes in molecules and clusters*". The first post is under the direction of Dr. Roy Johnston, and involves the use of a genetic algorithm to couple empirical and *ab initio* quality potential energy surfaces for clusters, to facilitate the search for accurate global minima and to develop reliable, but rapidly calculated, potential energy surfaces for the study of dynamic processes in clusters. This methodology will be used to study metallic, ionic and molecular clusters. The second post is in the group of Prof. Peter Knowles, and is in the area of molecular electronic structure method development. New computational methodology for *ab initio* calculations on large molecules will be designed and implemented.

The successful candidates will have a Ph.D. in theoretical chemistry or a related discipline, and will have proven ability to develop scientific software. Experience in the specific project areas is desirable. Under the terms of the EC programme supporting these posts, successful applicants must be aged 35 years or less, and must be nationals of a Community Member State or a state associated with the EC programme. UK nationals, or those who have carried out their normal activities in the UK for more than 12 of the 24 months prior to appointment, are ineligible.