Professor Roy Johnston BA, MA, DPhil, FRSC, CChem

Professor of Computational Chemistry
Deputy Head of School

School of Chemistry (/schools/chemistry/index.aspx)

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About

Roy Johnston is Professor of Computational Chemistry and Deputy Head of School. He is the School's Director of Research, Chair of the Postgraduate Research Committee of the College of Engineering and Physical Sciences and represents the College on the University's Graduate School Management Board. He is also a member of the Research Computing Management Board.

Roy has published over 150 research papers in scientific journals as well as reviews and book chapters in the fields of computational nanoscience and applications of nature-inspired computation. He has also authored a book “Atomic and Molecular Clusters” (2002) and edited several volumes and special issues of journals.

He has received major grants from EPSRC (including a Programme Grant of approximately £2.5M) and the Leverhulme Trust and is on the Management Committee of an EU COST Action on nanoalloys.

Research Webpages (http://www.tc.bham.ac.uk/~roy/)

Qualifications

- DPhil in Chemistry, Oxford University 1987
- BA (Hons, 1st class) in Chemistry, Oxford University 1983
- Fellow of the Royal Society of Chemistry (FRSC), 2003
- Chartered Chemist (CChem), 1990

Biography

Roy Johnston received his BA (1983) and D.Phil. (1986) from the University of Oxford, where he was a member of St. Catherine's College. His D.Phil., on theoretical aspects of cluster molecules, was carried out under the supervision of Professor Mike Mingos, FRS. From 1987-89, he was a SERC/NATO postdoctoral fellow in the U.S.A., spending a year each at Cornell University (working with Professor Roald Hoffmann (Nobel laureate) on theoretical solid state chemistry) and the University of Arizona (working with Professor Dennis Lichtenberger on gas phase and surface photoelectron spectroscopy).

He returned to the U.K. in 1989 as a Royal Society University Research Fellow at the University of Sussex, where he collaborated with Professor John Murrell on the development and application of many-body potentials for modelling clusters, surfaces and solids. He was appointed to a lectureship in inorganic chemistry at the University of Birmingham in 1995 and was promoted to senior lecturer in 2002 and reader in 2003. He was appointed Professor of Computational Chemistry in 2006.

Roy's research spans the fields of computational nanoscience and nature-inspired computation. Examples include the study of elemental and bimetallic clusters, the application of genetic and other nature-inspired algorithms to optimisation problems in chemistry and physics (e.g. protein folding, self-assembly, nanoparticle structure optimisation and structure solution from powder X-ray diffraction data), and developing techniques for visualising and analysing the complexity of energy landscapes. He is a Fellow of the Royal Society of Chemistry and is a past secretary of the RSC Theoretical Chemistry Group

Teaching

Teaching Programmes

- CHM2S6 - 2nd Year Introductory Computational Chemistry (Quantum Chemistry)
- CHM3E4 - 3rd Year Advanced Computational Chemistry (Computer Simulation)
- CHM4M3-I – Masters level Metal Clusters & Nanoalloys
- CHM4M3-II – Masters level Symmetry & Spectroscopy of Polyatomic Molecules

Postgraduate supervision

Current Group

- Chris Heard (1st year PhD)
- Ramli Ismail (3rd year PhD)
- Paul Jennings (2nd year PhD)
- Andy Logsdail (3rd year PhD)

- Dr Mark Oakley (PDRA)
- Paul West (3rd year PhD)

Roy is interested in supervising doctoral research students in the following areas:

- Modelling the structures, dynamics and reactivity (including catalytic activity) of bimetallic nanoalloy clusters.
- Exploring and analysing energy landscapes for protein folding and aggregation and other self-assembly processes.
- Chemical applications of natural computation.

Research

RESEARCH THEMES & ACTIVITY

Computational Nanoscience

- Development and application of many-body atomistic potentials to simulate the structures and growth patterns of metal, semiconductor and ionic clusters and nanoparticles. Development of Monte Carlo, Molecular Dynamics and Genetic Algorithm codes for global geometry optimization of cluster structures. Combining atomistic potentials and Density Functional Theory calculations to study bimetallic "nanoalloy" clusters which have important applications in heterogeneous catalysis (e.g. in catalytic converters in motor cars) as well as in electronics and for optical and magnetic applications. Study of free and surface-supported nanoparticles and simulation of electron microscopy images, surface plasmon spectra and EXAFS of metal nanoparticles and nanoalloys.
- This work has been supported by a grant of **£522,914** from EPSRC (EP/G070326/1) "Towards an Atomic-scale Understanding of the 3D Structure of Size-selected Clusters on Surfaces" (2009-13; with Z. Y. Li & R. E. Palmer (Physics, Birmingham) and J. Yuan (York)). Other support includes grants of over 300,000 cpu hours of computer time on national (the EPSRC *National Service for Computational Chemistry Software*) and international (HPC-Europa at Bologna, Helsinki and Edinburgh) facilities. Member of the EPSRC-funded *HPC Materials Chemistry Consortium*, with associated time on the UK's HPCx and HECToR supercomputers.
- Work in the area of cluster science has led to over 30 papers in international journals since 2001 as well as leading to the invitation to write a book ("Atomic and Molecular Clusters" - published by Taylor and Francis in April 2002) and invited ("Perspective") reviews (2003 and 2008) in two of the premier journals of the Royal Society of Chemistry. Co-author of a major review article on nanoalloys (published in *Chemical* Reviews in 2008). Chairman of the Royal Society of Chemistry *Faraday Discussion Meeting* on "Nanoalloys", held at the University of Birmingham from 3-5 September 2007. Editor of the volume of *Faraday Discussions* arising from this meeting (2008).

Nature-Inspired Computational Chemistry

- Development and application of Genetic Algorithms, Artificial Neural Networks, Ant Colony Optimization and Artificial Immune Systems for a variety of chemical problems.
- Editor of a volume of *Structure and Bonding* on "Applications of Evolutionary Computation in Chemistry" (published by Springer-Verlag in 2004).

Theoretical Chemical Biology

- Application of techniques developed for previous studies of clusters to study the protein folding problem.
- Investigation of potential energy hypersurfaces for protein folding and at new ways of visualising and analyzing the topologies and complexities of these surfaces.
- This work has been supported by a Wellcome Trust VIP grant; Royal Society UK-Japan Joint Research Project Grant and JSPS funding.

Theoretical Study of Self-Assembly

- **£2.62M (FEC = £3.18M)** has recently been awarded by EPSRC (EP/I001352/1) for the Programme Grant "Simulation of Self-Assembly" (20010-15; with D. Frenkel, D. J. Wales & M. A. Miller (Cambridge) and J. P. K. Doye (Oxford)).
- Systems to be studied include: protein folding and aggregation; RNA and DNA architectures; colloids and liquid crystals.
- The Birmingham component of the Programme, involves research into hybrid global optimization and developing methods for visualising and performing complexity analysis of potential and free energy landscapes.

Theoretical Structural Chemistry

- Development of a novel method for the *ab initio* solution of crystal structures from powder diffraction data, using a Genetic Algorithm.
- Application to solve the structures of a number of complex molecular solids, including some of the most complex molecules so far to be completely solved from powder diffraction data.
- Solution of the structures of a number of oligopeptides which have relevance for the study of hydrogen-bonding interactions in proteins and complex solids with several molecules in the asymmetric unit.
- Publication of over 30 papers and reviews.
- This research has received funding from EPSRC: SRIF funding for a Beowulf computer cluster; 3-year EPSRC research grant for a postdoctoral research fellow

Other activities

External Examiner (Masters Programmes)

- Warwick University, MSc in Scientific Computation (2011-)
- University of Oxford, MSc in Theoretical Chemistry (2009-)

External Examiner (PhD Theses)

- 2010 - University College London; Birkbeck College London; Sheffield University; University of Valladolid, Spain; University of Kiel, Germany.
- 2007 - Cambridge University; University of Genoa, Italy
- 2006 - Cambridge University; Loughborough University
- 2004 - University College London (2); University of Nottingham
- 2003 - Oxford University; Heriott-Watt University; University of Sussex; Bharathidasan University, Tiruchirappalli, India; Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India
- 2000 - Oxford University; University of Greenwich
- 1999 - Oxford University
- 1998 - Cambridge University

- 1993 - University of Rennes, France

Refereeing Grant Proposals

- Swiss National Supercomputing Grants (2010)
- Nuffield Research Bursaries (2009-)
- Austrian Science Foundation (2006)
- Cambridge University Research Fellowships (2006-)
- National Science Foundation (USA) (2005-)
- Marsden Fund (New Zealand) (2003)
- Member of EPSRC Chemistry Peer Review College (2000-)
- Leverhulme Trust Research and Fellowship Grant Proposals (1999-)
- STINT (Sweden) (1999)
- Royal Society Fellowship and Grant Proposals (1999-)

Conference Organisation

- Co-organiser of one day meeting: **Inorganic Chemistry at the Heart of England**, University of Birmingham (27 March 1996).
- Co-organiser of Royal Society Discussion Meeting: **The Metal-Non Metal Transition in Macroscopic and Microscopic Systems**, The Royal Society, London (5-6 March 1997).
- Organiser of CIBA Foundation Discussion Meeting: **Metal-Non Metal Transitions in Reduced Dimensions**, The CIBA Foundation, London (7 March 1997).
- Organiser of CCP5 Annual General Meeting 1999: **Simulation of Clusters and Interfaces**, University of Birmingham (6-8 September 1999).
- Director of Royal Society of Chemistry Theoretical Chemistry Group Summer School 2000: **Theory and Simulation of Clusters and Nanoparticles**, University of Birmingham (29 August - 6 September 2000).
- Organizer of 2 half-day meetings per year as Secretary of the Theoretical Chemistry Group of the Royal Society of Chemistry. (Final year postgraduate student lectures in March. *Theoretical Chemistry Day* at University College, London in December) (2002-05).
- Chief organiser of conference: **Modelling of Materials: Atomistic and Ab Initio Approaches**, Mansfield College, Oxford (9-10 April 2003).
- Organiser of meeting: **Theoretical and Experimental Inorganic Chemistry** (A Meeting to Celebrate the 60th Birthday of Professor D. Michael P. Mingos, FRS), St. Edmund Hall, Oxford (21 August 2004).
- Chairman of RSC **Faraday Discussion Meeting 138: Nanoalloys: From Theory to Applications**, University of Birmingham (3-5 September 2007).
- Member of International Scientific Committee for **III International Physics Congress**, University of Sonora, Hermosillo, Mexico (10-12 October 2007).

Editing

- Editor of *Double Vision* (the daily chemistry newsletter for the 1996 British Association for the Advancement of Science Festival - held at the University of Birmingham) 9-13 September 1996.
- Co-editor of published proceedings of Royal Society Discussion Meeting: **The Metal-Non Metal Transition in Macroscopic and Microscopic Systems** (*Phil. Trans. R. Soc. Lond. A* **1998**, *356*).
- Editor of Volume: **Applications of Evolutionary Computation in Chemistry** (*Struct. Bond. , Springer-Verlag, Heidelberg,* ***2004****, 110, ISBN: 3-540-40258-6).* , Springer-Verlag, Heidelberg,, , ISBN: 3-540-40258-6).
- Co-editor of published proceedings of **Faraday Discussion 138 – Nanoalloys: From Theory to Application** (*Faraday Disc.* **2008***, 138,* ISBN: 0-85404-119-2).
- Co-editor of book: *Nanoparticles* (In the Elsevier Series *Frontiers of Nanoscience*) (to appear in **2011**).

Miscellaneous

- Member of Management Committee and Leader of Work Group 1: Nanoalloy Phase Diagrams - **COST Action MP0903 "NANOALLOY - Nanoalloys as Advanced Materials: From Structure to Properties and Applications" (http://www.nanoalloy.eu/)** (2010-).
- Secretary & Treasurer - Royal Society of Chemistry **Theoretical Chemistry Group (http://www.rsc.org/tcg)** (2002-2005).
- Executive Committee Member - CCP5 (1999-2002).

Publications

- “Study of 40-atom Pt-Au Clusters Using a Combined Empirical Potential-Density Functional Approach" D. T. Tran and R. L. Johnston Proc. Roy. Soc. A **2011**, *2131*, 2004-2019“
- “Theoretical and Experimental Studies of the Optical Properties of Conjoined Gold-Palladium Nanospheres” A. J. Logsdail, N. J. Cookson, S. L. Horswell, Z. W. Wang, Z. Y. Li and R. L. Johnston *J. Phys. Chem. C* ***2010****, 114,* 21247-21251.
- “The Effect of CO and H Chemisorption on the Chemical Ordering of Bimetallic Clusters” P. S. West, R. L. Johnston, G. Barcaro and A. Fortunelli *J. Phys. Chem. C* **2010**, *114*, 19678-19686.
- “Theoretical Study of $Cu_{38-n}Au_n$ Clusters Using a Combined Empirical Potential/Density Functional Approach” T. D. Tran and R. L. Johnston *PhysChemChemPhys* **2009**, *11*, 10340-10349.
- “Theoretical Studies of Palladium-Gold Nanoclusters: Pd-Au Clusters with up to 50 Atoms” F. Pittaway, L. O. Paz-Borbón, R. L. Johnston, H. Arslan, R. Ferrando, C. Mottet, G. Barcaro and A. Fortunelli *J. Phys. Chem. C* ***2009****, 113,* 9141-9152.
- “Structural Motifs, Mixing and Segregation Effects in 38-atom Binary Clusters” L. O. Paz-Borbón, R. L. Johnston, G. Barcaro and A. Fortunelli *J. Chem. Phys.* **2008**, *128*, 134517.
- “Nanoalloys: From Theory to Applications of Alloy Clusters and Nanoparticles” R. Ferrando, J. Jellinek and R. L. Johnston *Chem. Rev.* **2008**, *108*, 845-910.
- “Searching for the Optimum Structures of Alloy Nanoclusters” (Invited Perspective) R. Ferrando, A. Fortunelli and R. L. Johnston *Phys. Chem. Chem. Phys.* **2008**, *10*, 640-649.
- “Energetic, Electronic and Thermal Effects on Structural Properties of Ag-Au Nanoalloys” F. Y. Chen and R. L. Johnston *ACS Nano* ***2008****, 2,* 165-175.
- “Three-dimensional Atomic-scale Structure of Size-selected Gold Nanoclusters” Z. Y. Li. N. P.Young, M. Di Vece, S. Palomba, R. E. Palmer, A. L. Bleloch, B. C. Curley, R. L. Johnston, J. Jiang and J. Yuan *Nature* **2008**, *451*, 46-48.
- “Structures and Energetics of 98-atom Pd-Pt Nanoalloys: Potential Stability of the Leary Tetrahedron for Bimetallic Nanoparticles” L. O. Paz-Borbón, T. V. Mortimer-

Jones, R. L. Johnston, A. Posada-Amarillas, G. Barcaro and A. Fortunelli *Phys. Chem. Chem. Phys.* ***2007***, *9,* 5202-5208.

- “Nanofinger Growth on Au(111) Arising from Kinetic Instability” N. Toto, R. Ferrando, Q. Guo and R. L. Johnston *Phys. Rev. B* ***2007***, *75,* 195434.
- “A Mixed Structural Motif in 34-atom Pd-Pt Clusters” L. O. Paz-Borbón, R. L. Johnston, G. Barcaro and A. Fortunelli *J. Phys. Chem. C* ***2007***, *111,* 2936-2941.
- “Topographical Complexity of Multidimensional Energy Landscapes” G. J. Rylance, R. L. Johnston, Y. Matsunaga, C.-B. Li, A. Baba and T. Komatsuzaki *Proc. Natl. Acad. Sci. USA* ***2006***, *103,*18551-18555.
- “Evolving Better Nanoparticles: Genetic Algorithms for Optimizing Cluster Geometries” (Dalton Perspective) R. L. Johnston, *Dalton Trans.* **2003**, 4193-4207.
- “Atomic and Molecular Clusters” R. L. Johnston: book in the *Masters Series in Physics and Astronomy* (series editor D. S. Betts)published by Taylor & Francis Ltd., London **2002** (ISBN 0748409319)