Professor Roy L Johnston

Professor of Computational Chemistry

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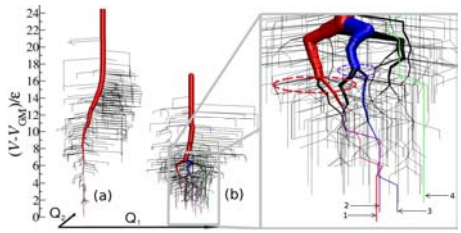
Keywords: *computational nanoscience, nature-inspired computation, energy landscapes, clusters, nanoalloys, protein folding*

Research Interests:

Computational Nanoscience: We develop and apply many-body atomistic potentials to optimise the structures and simulate the growth patterns, chemical ordering and dynamics of metal (including bimetallic "nanoalloys"), semiconductor and ionic clusters, employing Monte Carlo, Molecular Dynamics and Genetic Algorithm codes.[1,2] We carry out Density Functional Theory calculations of the electronic structures of metallic and bimetallic clusters.[3] As part of a collaboration with Professor Richard Palmer and Drs Ziyou Li and Quianmin Guo in the Nanoscale Physics Research Laboratory, School of Physics & Astronomy, we simulate STEM images of surface-deposited mono- and bimetallic clusters[4] and model nanofinger formation on Au surfaces.[5] ***Nature-Inspired Computational Chemistry:*** We develop and apply Genetic Algorithms, Artificial Neural Networks, Ant Colony Optimization and Artificial Immune Systems for a variety of chemical problems, ranging from cluster geometry optimization[6] to protein folding[7] and structure solution from powder X-ray diffraction data.[8] ***Investigation of Energy Landscapes:*** *We develop* methods for visualising and analysing the complexity of energy landscapes – e.g. for protein folding and cluster rearrangement.[9]

The Leary tetrahedron – identified as a potentially stable structure for 98-atom nanoalloy clusters.[1]



2D metric disconnectivity graphs for two model proteins.[9]

Recent Publications

1. L. O. Paz-Borbón, T. V. Mortimer-Jones, R. L. Johnston, A. Posada-Amarillas, G. Barcaro, A. Fortunelli, *Phys. Chem. Chem. Phys.* 2007, **9**, 5202-5208.
2. F. Y. Chen, B. C. Curley, G. Rossi, R. L. Johnston, *J. Phys. Chem. C* 2007, **111**, 9157-9165.
3. L. O. Paz-Borbón, R. L. Johnston, G. Barcaro, A. Fortunelli, *J. Phys. Chem. C* 2007, **111**, 2936-2941.
4. B. C. Curley, R. L. Johnston, N. P. Young, Z. Y. Li, M. Di Vece, R. E. Palmer, A. L. Bleloch, *J. Phys Chem. C* 2007 (in press).
5. N. Toto, R. Ferrando, Q. Guo, R. L. Johnston, *Phys. Rev. B* 2007, **75**, 195434.
6. R. L. Johnston, *Dalton Trans.* 2003, 4193-4207.
7. G. A. Cox, T. V. Mortimer-Jones, R. P. Taylor, Roy L. Johnston, *Theor. Chem. Acc.* 2004, **112**, 163-178.
8. S. Habershon, E. Y. Cheung, K. D. M. Harris, R. L. Johnston, *J. Phys. Chem. A* 2004, **108**, 711-716.
9. G. J. Rylance, R. L. Johnston, Y. Matsunaga, C.-B. Li, A. Baba, T. Komatsuzaki, *Proc. Natl. Acad. Sci. USA* 2006, **103**, 18551-18555.