

**Dr Paul Martin** BSc(Hons.), MSc, PhD

Research Fellow

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## About

Dr Paul Martin joined the School of Geography, Earth and Environmental Sciences at Birmingham as a Research Fellow working with Professor Valsami-Jones on the ModNanoTox project to model nanoparticle toxicity to describe the behaviour of engineered nanoparticles in organisms and the environment. The main objective of Paul's work is to develop molecular models of surface reactivity of nanoparticles, thus creating the mechanistic basis to link reactivity with toxicity.

## Qualifications

- PhD Computational Chemistry
- MSc Multidisciplinary Bio-Informatics
- PGCE (Science – Chemistry)
- BSc (Hons.) Combined Science – Chemistry and Computer Science

## Biography

After teaching chemistry at key stages 3, 4 and 5, Dr Martin won a scholarship to study for an MSc in Bioinformatics at Leeds University and later joined the Computational Solid State Chemistry group at Bath University to do a PhD in atomistic modelling of the structure and reactivity of ionic nanoparticles under the supervision of Professor S.C. Parker. Dr Martin was then a Marie Curie Host Post-doctoral Fellow at Trinity College Dublin, again modelling materials at the nanoscale. Returning to England, Dr Martin took a temporary chemistry lectureship at Nottingham-Trent University, and was employed through the RSC administered 'Chemistry for our Future' project and carried out pedagogical research developing and presenting various approaches to undergraduate level chemistry teaching, and lectured aspects of materials, biological and environmental chemistry. On completion of the project Dr Martin worked as a Research Fellow at Huddersfield University where he worked on concurrent projects involving modelling biomineralisation and also investigating the suitability of thorium as a nuclear fuel. Dr Martin also works as an Associate Lecturer with the Open University where he tutors for the Level 3 Chemical Change and Environmental Applications module.

## Research

### Research interests

- Computational Chemistry
- Nanoscale Materials Modeling
- Solid State Chemistry particularly Minerals and their Surfaces
- Modelling Biomineralisation
- Modelling Nanotoxicity and Reactivity

## Publications

Martin, P., Cooke, D. and Cywinski, R. (2012) '**[A molecular dynamics study of the thermal properties of thorium oxide](http://eprints.hud.ac.uk/15443)**' *Journal of Applied Physics* , **112 (7)**, p. **073507**. ISSN **0021-8979** (<http://eprints.hud.ac.uk/15443>) , 112 (7), p. 073507. ISSN 0021-8979

'Computer Modelling of Thorium: Determining the Suitability of Thorium as a Next Generation Nuclear Fuel' In: UNTF 2011: Universities Nuclear Technology Forum. The University of Huddersfield 11th -13th April, 2011.

Testing Interatomic Potentials for QM/MM Embedded-Cluster Calculations on Ceria Surfaces. Paul Martin, Natasha M. Galea, David O. Scanlon, Graeme W. Watson, and Paul Sherwood. E-journal of Surface Science and Nanotechnology. 7, 413-420 (2009).

Defect Ceria Surfaces: Comparing Interatomic Potentials with Density Functional Theory. Paul Martin, Natasha M. Galea, David O. Scanlon and Graeme W. Watson. Theoretical Aspects of Catalysis, eds. G. Vayssilov, T. Mineva, Heron Press, Sofia, 2009.

The Changing Shape of Chemistry, 1998 to 2008. Paul Martin and Karen Moss. Chemistry World, April Issue, 2009.

'Unlocking the Oxygen Storage Capacity of Ceria – a Research-Linked Learning Resource and Activity.' In: Research-Teaching Links in the Physical Sciences: Politics and Practise. HEA Physical Science Professional Development Workshop. University of Warwick, 2009.

Developments across the curriculum: problem-based and context-based learning resources within the chemical curriculum at NTU. Paper In: Proceedings of the Science Learning and Teaching Conference. Developments in Learning and Teaching – Forward Thinking, [O9] 16-17 June 2009, Heriot-Watt University, Edinburgh (2009).

Atomistic Modelling of Multilayered Ceria Nanotubes Paul Martin, Stephen C. Parker, Dean C. Sayle, and Graeme W. Watson. Nanoletters, Vol. 7, No. 3, (2007) pp. 543-

Application of molecular dynamics DL\_POLY codes to interfaces of inorganic materials. Martin P., Parker S.C., Sayle D.C., Spagnoli D., Watson G.W. Marmier A., Molecular Simulation, Vol. 32, Nos. 12–13, 15 October–15 November 2006, 1079–1093

Modelling the structure and transport at mineral interfaces at the atomic level. Parker S.C., Cooke D.J., Marmier A., Martin P., Spagnoli D., Sayle D.C. and Watson G.W. Geochemical et Cosmochemica Acta 79, A471 (2006)

Computer Modelling of Oxygen Mobility at Ceria Surfaces and the Construction of Ceria Nanotube Models. Martin P., Parker S.C., Sayle D.C., Watson G.W. Advances in Science and Technology 46, 48-53, (2006).

Computer Modelling of Oxygen Mobility at Ceria Surfaces and the Construction of Ceria Nanotube Models. In: Abstracts of papers of the 11th International Ceramics Congress & 4th Forum on New Materials, CIMTEC 2006.

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