University of Birmingham

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Senior Lecturer in Computational Solid State Chemistry

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About

Dr Mark S D Read is a Senior Lecturer in the area of computational solid state materials chemistry whose research interests cover a range of subjects within contemporary materials chemistry modelling, with particular focus on the deployment and development of atomistic simulation methodologies to extend our understanding of the structure, stability and reactivity of solid state materials at the atomic level, particularly those with relevance to industrial and energy applications.

In addition to teaching Physical Chemistry within the School of Chemistry, Mark is also part of the Birmingham Centre for Nuclear Education and Research and contributes to the following MSc programmes:

- **Nuclear Decommissioning and Waste Management (/postgraduate/courses/taught/gees/nuclear-decommissioning.aspx)**
- **Physics and Technology of Nuclear Reactors (/postgraduate/courses/taught/physics/physics-technology-nuclear-reactors.aspx)**

In addition, he is actively engaged in promoting research to support the UK's investment in nuclear power generation.

Qualifications

- Fellow of the Royal Society of Chemistry, 2010
- Chartered IT Professional of the British Computer Society, 2007
- PhD in Computational Chemistry, University of Surrey, 1999
- Chartered Membership of the Royal Society of Chemistry, 1998
- BSc (Hons) in Chemistry, University of Surrey, 1992

Biography

Mark Read obtained his BSc (Hons) in Chemistry at the University of Surrey and, after spending three years in industry as an Occupational Health and Environmental Consultant, studied for his PhD at the University of Surrey as a CASE Student with Industrial Sponsor ICI Katalco on the topic: “Atomistic Simulation Studies of the Defect and Surface Properties of Perovskite-based Oxide Catalysts” which lead to improved formulation of the Hydecat™ catalyst.

Mark was granted Chartered status within the Royal Society of Chemistry in 1998 and has subsequently become a Chartered Scientist (2004) with the Science Council and more recently a Chartered IT Professional with the British Computer Society (2007) before being elected to a Fellowship of the Royal Society of Chemistry in 2010.

After completion of his PhD in 1999, Mark undertook industrial research within the defence industry establishing a chemical modelling capability which complemented materials ageing research programmes with fundamental simulation studies. Mark left the Research and Applied Science Directorate as a Principal Scientific Officer and Team Leader for the Computational Chemistry Team in 2012 for a senior lectureship appointment in the School of Chemistry at the University of Birmingham and is a member of and is a member of the Centre for Nuclear Education and Research.

Teaching

Teaching Programmes

- Physical Chemistry for Chemical Engineers
- Year 1 Mathematics for Chemists

Nuclear Decommissioning and Waste Management MSc

- Waste Processing and Treatment
- Encapsulation

Postgraduate supervision

- Atomistic simulation of nuclear fuels
- Atomistic simulation of candidate matrices for high level waste encapsulation
- Computer modelling of radiation damage

For a full list of available Doctoral Research opportunities, please visit **the School of Chemistry website (/schools/chemistry/index.aspx)** .

Research

Research themes

The Read group undertakes research in Computational Solid State Materials Chemistry, with interests in civil nuclear fuels (actinide oxides), candidate matrices for high level waste encapsulation and simulating radiation damage in materials of interest. Underpinning all our research is the deployment and development of atomistic simulation methodologies to extend our understanding of the structure, stability and reactivity of these solid state materials at the atomic level.

Research activity

Atomistic simulation of civil nuclear fuels

Current activity includes the simulation of ageing effects on nuclear fuels (uranium and plutonium oxides), radiation damage and modelling the defect chemistry within the bulk and at surfaces (which control many important material properties). Indeed, the corrosion of nuclear fuels is an extremely pertinent area of research and is crucial to the safety and sustainability of the nuclear fuel cycle.

Atomistic simulation of candidate matrices for high level waste encapsulation

Nuclear energy research in the UK is currently undergoing a renaissance due to the need to reduce the reliance on carbon-based fuels and to meet the country's long term CO2 emission reduction commitments. New reactors are planned to replace existing plant but there is considerable public scepticism especially concerning safety and waste storage. It is thus important to demonstrate the effectiveness of current waste storage methods when products remain active over many years and to develop improved methods.

Publications

Littleford TE, Jackson RA and Read MSD, (submitted 2012), "An atomistic surface simulation study predicting morphologies and segregation in Yttrium Lithium Fluoride", **Surface Science** – tbd

Letant SE, Plant DF, Wilson TS, Alviso CT, Read MSD and Maxwell RS, (2011), "Application of density functional theory to the investigation of polymer degradation: Example of cross-linked ethylene-vinyl acetate-vinyl alcohol (EVA-OH) terpolymer de-acetylation", **Polymer Degradation and Stability**, 96: 2019-2028

Read MSD and Jackson RA, (2010), "Derivation of enhanced potentials for uranium dioxide and the calculation of lattice and intrinsic defect properties", **Journal of Nuclear Materials**, 406: 293–303

Allen JP, Parker SC and Read MSD, (2009), "Using atomistic simulation to study the interaction of water and carbonate with oxide surfaces**", Geochimica et Cosmochimica Acta**, 73: A29

Read MSD, Islam MS, Watson GW and Hancock FE, (2001), "Surface structures and defect properties of pure and doped La2NiO4", **J. Mater. Chem.**, 11: 2597–2602

Read MSD, Islam MS, Watson GW, King F and Hancock FE, (2000), "Defect chemistry and surface properties of LaCoO3", **J. Mater. Chem.**, 10: 2298-2305

Read MSD, Islam MS, King F and Hancock FE, (1999), "Defect Chemistry of La2Ni1-xMxO4 (M = Mn, Fe, Co, Cu): Relevance to Catalytic Behavior", **J. Phys. Chem. B**, 103, 1558-1562

Islam MS, Read MSD and D'Arco S, (1997), "From oxides to oxyhalides: modelling the properties of high T-c superconductors", **Faraday Discussions**, 106: 367-376