

Structural Chemistry of Functional Materials: Hops and Twists in the Solid State

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An in-depth understanding of the structure – property relationships is essential for the successful discovery and preparation of new functional materials capable of overcoming the limitations of the currently used ones. As materials' complexity increases, structural characterisation using a range of scattering-based and complementary techniques and state-of-the-art data analysis approaches, aided by computational simulations, is essential in providing this insight.

This presentation will give an overview of the recent work carried out in the IRE group in several areas of functional materials research: the elucidation of key motifs, defects and mechanisms giving rise to ionic mobility in materials for energy applications;^{1,2} the development of advanced structural data analysis methodologies capable of tackling exceptionally complex crystallographic problems arising from phase transitions;³ the complementary use of long-range and local structural probes in understanding the properties and disorder in functional solids across the chemical spectrum, from energy- to pharmaceutically-relevant materials.^{4,6}

References:

1. *New Apatite-Type Oxide Ion Conductor, $\text{Bi}_2\text{La}_8[(\text{GeO}_4)_6]\text{O}_3$: Structure, Properties and Direct Imaging of Low-Level Interstitial Oxygen Atoms using Aberration-Corrected Scanning Transmission Electron Microscopy*, M. L. Tate, D. A. Blom, M. Avdeev, H. E. A. Brand, G. J. McIntyre, T. Vogt and I. Radosavljevic Evans, [Advanced Functional Materials, 27, 8, 1605625, 2017.](#)
2. *Remarkably High Oxide Ion Conductivity at Low Temperature in an Ordered Fluorite-Type Superstructure*, X. Kuang, J. L. Payne, M. R. Johnson and I. Radosavljevic Evans, [Angewandte Chemie International Edition, 51, 690, 2012.](#)
3. *An Exhaustive Symmetry Approach to Structure Determination: Phase Transitions in $\text{Bi}_2\text{Sn}_2\text{O}_7$* , J. W. Lewis, J. L. Payne, I. Radosavljevic Evans, H. T. Stokes, B. J. Campbell, and J. S. O. Evans, [Journal of the American Chemical Society, 138, 25, 8031, 2016.](#)
4. *A Furosemide–Isonicotinamide Cocrystal: An Investigation of Properties and Extensive Structural Disorder*, H. E. Kerr, L. K. Softley, S. Kuthuru, A. Nangia, P. Hodgkinson and I. Radosavljevic Evans, [CrystEngComm, 17, 6707, 2015.](#)
5. *On $\text{Sr}_{1-x}\text{Na}_x\text{SiO}_{3-0.5x}$ New Superior Fast Ion Conductors*, I. Radosavljevic Evans, J. S. O. Evans, H. G. Davies, A. R. Haworth and M. L. Tate, [Chemistry of Materials, 26, 18, 5187, 2014.](#)
6. *Na^+ Mobility in Sodium Strontium Silicate Fast Ion Conductors*, J. R. Peet, C. M. Widdifield, D. C. Apperley, P. Hodgkinson, M. R. Johnson and I. Radosavljevic Evans, [Chemical Communications, 51, 17163, 2015.](#)

Ivana Radosavljević Evans Curriculum Vitae



Grenoble

Ivana Radosavljević Evans was born in [Belgrade](#), the capital of [Serbia](#). She obtained her first degree in Physical Chemistry at the University of Belgrade in 1992. In 1995 she enrolled in the postgraduate program in Chemistry at Oregon State University and worked under the supervision of Professor Art Sleight. She obtained her PhD degree in 1998. After moving to the UK, she joined the group of Professor Judith Howard at the [Durham University Department of Chemistry](#) as a post-doctoral research associate. She was the recipient of the Cambridge Crystallographic Data Centre Prize for Younger Scientist Award for 2003. In 2005, she took up an RCUK Academic Fellowship. She was appointed a Lecturer in in Structural/Materials Chemistry in 2009, promoted to Senior Lecturer in 2011 and [Reader](#) in 2015.

The research interests and activities in the [IRE group](#) are in the area of solid state chemistry and structure-property relationships of functional materials. The projects encompass synthetic work (solid state, soft chemistry, crystal growth), characterisation of structure and dynamics (powder and single crystal X-ray and neutron diffraction, electron microscopy, total scattering, solid state NMR, inelastic/quasi-elastic neutron scattering), determination of physical properties (impedance spectroscopy, photocatalytic activity measurements, luminescence) and computational modelling (ab-initio molecular dynamics).

Ivana was the Chair (2011-2014) of the Physical Crystallography Group of the British Crystallographic Association and the Structural Condensed Matter Physics Group of the Institute of Physics. She has served on the Diffraction peer review panel for Diamond Light Source (2010-2014) and is currently a member of the ISIS Diffraction peer review panel and the Royal Society of Chemistry Materials Chemistry Division Council. At Durham Chemistry, she is the leader of the [Functional Molecules and Materials Research Grouping](#).

Her up-to-date publication list is available at [Google Scholar](#).