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Design and Discovery of Functional Materials – Synthesis, Structure, Computation and Machine Learning

This presentation will cover our recent work on digital routes to new materials realised in the laboratory. It will address the roles of machine learning and structure prediction in targeting materials where new structures, rather than those already in the databases, give high performance. (Angewandte Chemie-International Edition. 2021, 60, 2–11).

This broader context leads to a focus on the synthesis of new multiple anion materials, including the distinctive structures accessible from the ordering of distinct formally negatively charged species (J. Am. Chem. Soc. 2017, 139, 44, 15568–15571; J. Am. Chem. Soc. 2020, 142, 2, 847–856). Properties will include low thermal conductivity (Science 373, 1017-1022, 2021) and structural families for lithium ion transport (Chem. Mater. 33, 2206-2217, 2021) and as sodium ion cathodes (J. Mater. Chem. A, 2020, 8, 20553-20569). The role of machine learning in supporting the search for new multiple anion systems will be discussed, using the example of stable interfaces to lithium in solid state batteries (Nature Communications 2021, 12, 5561).

Matthew Rosseinsky obtained a degree and a D. Phil in Chemistry from the University of Oxford in 1990. He was a Postdoctoral Member of Technical Staff at A.T.&T. Bell Laboratories then in 1992 was appointed University Lecturer in Chemistry at the University of Oxford. In 1999 he moved to the University of Liverpool as Professor of Inorganic Chemistry. He was elected a Fellow of the Royal Society in 2008, and was awarded the Hughes Medal of the Royal Society in 2011. In 2013 he became a Royal Society Research Professor. He was awarded the inaugural de Gennes Prize for Materials Chemistry (a lifetime achievement award open internationally) by the Royal Society of Chemistry in 2009, the C.N.R. Rao Award of the Chemical Research Society of India in 2010 and gave the Muetterties Lectures at UC Berkeley and Lee Lectures at the University of Chicago in 2017. He was awarded the Davy Medal of the Royal Society in 2017. He was a member of the governing Council of the Engineering and Physical Sciences Research Council from 2015 - 2019. His work addresses the synthesis of new functional materials in bulk and thin film form for energy, catalysis and information storage applications, and has been characterised by extensive collaboration with many academic and industrial colleagues, together with an integrated computational and experimental approach to materials discovery. Current areas of interest include materials for batteries and solid oxide fuel cells, multiferroics, thermoelectrics, superconductivity, materials for separations and catalysis, high-throughput materials discovery, and materials for solar energy conversion.