



COLLÈGE
DE FRANCE
—1530—

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DESIGN OF ADVANCED MATERIALS ?

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The development of advanced materials will increasingly rely on our ability to assemble complex compositions in an ordered and predictable manner to generate enhanced properties. It is attractive to harness the ever-increasing power of computation in the search for new materials, but the scale and nature of the problem make brute force de novo approaches challenging, while “big data” searches for analogues of existing structures in databases cannot identify potentially transformative new structures. Building chemical knowledge into computational tools used together with experiment offers a different approach. I will present an example of crystal chemically-informed computational identification of a new solid oxide fuel cell cathode (1). This integrated approach has recently allowed

us to combine permanent magnetism and electrical polarisation in a single phase material above room temperature (2), a major challenge in materials synthesis because of the competing electronic structure requirements of these two ground states. As a counterpoint, we have recently used a non-computational multiple length scale symmetry control strategy to switch both of these long-range orders in a magnetoelectric multiferroic at room temperature (3). This emphasises the enduring importance of developing the crystal chemical understanding that drives “classical” approaches to materials design.

- (1) M. Dyer et al Science 340, 847, 2013
- (2) M. Pitcher et al Science 347, 420, 2015
- (3) P. Mandal et al Nature 525, 363, 2015

Matthew Rosseinsky obtained a degree in Chemistry from the University of Oxford and a D. Phil under the supervision of Professor P. Day, FRS in 1990. He was a Postdoctoral Member of Technical Staff at A.T.&T. Bell Laboratories in Murray Hill, New Jersey where his work with D.W. Murphy, A.F. Hebard and R.C. Haddon led to the discovery of superconductivity in alkali metal fullerenes. In 1992, he was appointed University Lecturer at the Inorganic Chemistry Laboratory, University of Oxford, where he remained until 1999 when he moved to the University of Liverpool as Professor of Inorganic Chemistry. He was awarded the inaugural de Gennes Prize for Materials Chemistry by the Royal Society of Chemistry in 2009 and the C.N.R. Rao Award of the Chemical Research Society of India in 2010. Elected a Fellow of the Royal Society in 2008, he was awarded the Hughes Medal of the Royal Society in 2011. In March 2013 he became a Royal Society Research Professor. He is a member of the UK Science Minister's Advanced Materials Leadership Council, and of the Council of the Engineering and Physical Sciences Research Council. His work addresses the synthesis of new functional materials for energy and information storage applications, and has been characterised by extensive collaboration with many academic and industrial colleagues.