EPFL Valais, ChE 602 Seminar, 22.06.2017

Title: Design of Advanced Materials ?

Abstract:

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. 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 and complementary approach. I will present an example of crystal chemically-informed computationally-enabled identification of a new solid oxide fuel cell cathode (1). By accelerating the structure prediction tools used in this study, we have been able to predict ab initio regions of composition space that afford new materials, and then isolate those materials experimentally: this approach promises to expedite the structure with new currently slow experimental realisation of new composites. 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. Design of coherent interfaces between materials with different crystal structures to permit layer-by-layer heterostructure growth is also discussed. (4)

(1) M. Dyer et al *Science* 340, 847, **2013**

(2) M. Pitcher et al *Science* 347, 420, **2015**

(3) M. O'Sullivan et al *Nature Chemistry* **8**, 347, **2016**

Bio:

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 fullerides. 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 (a lifetime award for achievement in this research area open to all scientists internationally) by the Royal Society of Chemistry in 2009 and the C.N.R. Rao Award of the Chemical Research Society of India in 2010. He was elected a Fellow of the Royal Society in 2008, and 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 Science

Minister’s Advanced Materials Leadership Council, and of the Council of the Engineering and Physical Sciences Research Council, the UK funding body for this area of research. 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.