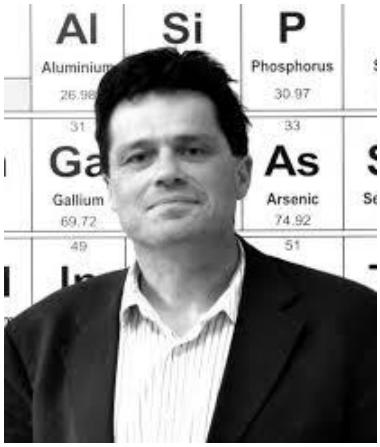
**Swiss Society for Crystallography**

**Howard Flack Crystallographic Lectures Series**

**Prof. Dr. Matthew J. Rosseinsky**
Department of Chemistry, University of Liverpool, Liverpool L69 7ZD, UK




Lecture Series:

# Design of Advanced Materials?

Monday, **4 November 2019, 14:15**
**Paul Scherer Institute**
PSI East, room OSGA/EG06 (in front of the OASE mensa), 5232 Villigen

Tuesday, **5 November 2019, 10:00**
**CSEM Neuchâtel**
Rue Jaquet-Droz 1, CH-2002 Neuchâtel

Wednesday, **6 of November 2019, 17:00**
**University of Fribourg**
Main auditorium, Chemistry Department, Chemin du Musée 9, 1700 Fribourg

Thursday, **7 November 2019, 17:15**
**EPFL Lausanne**
Auditorium BCH 2201, ISIC, Station 6, 1015 Lausanne

Friday, **8 November 2019, 11:00**
**Empa in Dübendorf**
VE102, Empa Dübendorf, 8600 Dübendorf, Überlandstrasse 129

# Abstract of the lecture series
# '**Design of Advanced Materials?**'

M.J. Rosseinsky
Department of Chemistry, University of Liverpool, Liverpool L69 7ZD, UK

The knowledge we have developed through the synthesis and experimental study of extended solids allows us to efficiently identify new materials, in many cases with scientifically interesting or technically important changes in properties. An example is the chemical control of the transparent conducting behaviour of correlated metals (1), evaluated as epitaxial films through optical and transport data. The selection of $d^0$ cations to stabilise oxygen-oxygen bond formation upon deep oxidation of lithium ion cathodes is a further example (2). Here computation provides underpinning guidance in the selection of experimental targets.

However, the large potential range of accessible compositions and structures challenges our present capabilities. As part of the current interest in exploring computationally-enabled routes to new materials, we are developing computational tools for the identification of stable new compositions. We have recently (3) been able to predict *ab initio* the regions of composition space that afford new materials, and then subsequently isolate those materials experimentally, using the computation of the energies of probe structures identified by new crystal structure prediction methods (4) to explore the space. The presentation will discuss the potential offered by informatics approaches often referred to as machine learning in such work.

(1) J.L. Stoner *et al.*, *Advanced Functional Materials* **29**, 1808609, 2019

(2) Z. Taylor et al., *J. Am. Chem. Soc.* **141**, 7333, 2019

(3) C. Collins *et al., Nature* **546**, 280-284, 2017

(4) C. Collins *et al.*, *Faraday Discussions* **211**, 117, 2018

# CV
## M.J. Rosseinsky

**Matthew Rosseinsky** obtained his undergraduate degree and D. Phil in chemistry from the University of Oxford. He was a postdoctoral member of the technical staff at AT&T Bell Laboratories before returning to the University of Oxford as a lecturer in chemistry. In 1999, he moved to the University of Liverpool as professor of inorganic chemistry. In 2009, Matthew received the inaugural De Gennes Prize from the Royal Society of Chemistry (RSC) — a lifetime achievement award in materials chemistry that is open internationally and is one of the RSC's three premier awards. He was elected a Fellow of the Royal Society in 2008, and was awarded the Hughes Medal of the Royal Society in 2011 for his highly influential discoveries in the synthetic chemistry of solid state electronic materials and novel microporous structures. In 2013, he became a Royal Society Research Professor, and was awarded its Davy Medal in 2017.

Matt's work addresses the synthesis of new functional materials in bulk and thin-film form for energy and information storage applications, and has been characterized by extensive collaboration with many academic and industrial colleagues. The Rosseinsky group's current areas of interest include materials for batteries and solid oxide fuel cells, multiferroics, thermoelectrics, superconductivity, materials for separation and catalysis, high-throughput materials discovery, and materials for solar energy conversion.

A central topic of Matt's research is the development of new methods of identifying functional materials, emphasising the integration of experiment with computational methods for materials discovery, which includes new tools for crystal structure prediction.

**https://www.liverpool.ac.uk/chemistry/research/rosseinsky-group/**