



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/>

Report on the 2019 Howard Flack Crystallographic Lecture Series

From 4th to 8th November 2019 it was our great pleasure to welcome Prof. Matthew Rosseinsky from the Department of Chemistry of the University of Liverpool, UK. He gave five lectures in the frame of our distinguished Howard Flack Crystallographic Lecture Series, which we established in 2018.



1 Matthew Rosseinsky lecturing at PSI

After arriving on Monday morning at Zurich airport, he started his Switzerland tour at the PSI in Villigen. Before his lecture in the afternoon, we had time for discussions with colleagues.

After Matt travelled by train to Neuchâtel, we enjoyed dinner at the Hotel 'Alpes et Lac' where he stayed for two nights and also profitted from a visit to downtown Neuchâtel. On Tuesday morning, Matt visited the research and technology organization CSEM, where a large audience of materials scientists,

researchers in micro and nano systems and from the energy and life science departments welcomed him. Matt was impressed by such a huge interest in his research topic and made an excellent presentation. Colleagues from the UniNE, UniGe and UniBe also came to CSEM to attend Matt's lecture. Prof. Rosseinsky had several discussions on the importance of computational investigations of interfaces (especially at the nanoscale), for the control of functional interfaces for medical diagnostics, single molecule electronics and for energy applications. By the end of the day, Matt underlined that he had had an outstanding scientific exchange at CSEM.



2 Exchange with students at the University of Fribourg

On Wednesday morning, he travelled by train through the 'Seeland' to Fribourg where the students of the Fromm group started discussions during the afternoon before his lecture in the late afternoon at the Department of Chemistry of the University of Fribourg.

In the evening, lively discussions continued with Katharina Fromm during dinner. The next morning, Matt's journey brought him to EPFL in Lausanne, where he arrived still very much in shape after the last three intense days and just in time for lunch, which was shared with colleagues while enjoying the view of the Lake of Geneva. Although the weather was lousy, spirits were high and the discussion with known and new colleagues was lively. A busy four-hour

afternoon schedule had been prepared for Matt to meet colleagues one-on-one, until shortly before he presented his Flack Lecture. A brief slot of 15 minutes to relax and prepare was enough for Matt to deliver an energetic and didactic lecture that was thoroughly enjoyed by students from EPFL and colleagues from the University of Geneva, who had made the trip for this occasion. The lecture was followed by an

apéro, after which Matt had to get back on the train, the next stop being Empa near Zurich, on the other side of Switzerland. It was a pleasure having Matt at EPFL.

After the long and intense day in Lausanne, Matt started early on Friday morning at Empa in Dübendorf. We initiated the day with lab visits at the Center for X-ray Analytics



followed by discussions with Empa colleagues. At 11am he started his talk at the Empa Academy, where we were fascinated by his lecture about his current interest in exploring computationally-enabled routes to new materials and the application of ML (machine learning) tools for the identification of stable new material compositions.

3 Matthew Rosseinsky' s lecture at the Empa Academy in Dübendorf

lively discussions between Matt and colleagues and friends from the ETHZ, the University of Zurich and, of course, Empa.

The lecture was followed by a lunch accompanied by



4 Lunch at Empa Dübendorf with Matt Rosseinsky and colleagues from the SSCr after the lecture

In the early afternoon, he returned to Zürich airport to catch his flight back to Liverpool. It has been a great experience and a real pleasure to welcome Prof. Matthew Rosseinsky here in Switzerland. We thank him very much for the fascinating lecture series and for accepting our dense travel and lecture schedule.

Pascal Schouwink, Olha Sereda and Antonia Neels