



ENI AWARD 2023

Energy Frontiers

Matthew Rosseinsky

Winner

Digital design and discovery of next-generation energy materials

Research Description

Matthew Rosseinsky works on the design and discovery of new materials. This involves both the development of materials for specific applications and the exploration of uncharted new chemistry, where we learn for the first time about the possible arrangements of atoms in materials, thus opening fresh paths to produce materials for application. Both these strands of work require the realisation in the laboratory of new materials. Since these are by definition without precedent, this is a challenging task, particularly given the astronomical number of possible atomic combinations and materials structures. In order to accelerate progress, Rosseinsky has developed a new approach to the discovery of materials that combines digital computational tools with experimental synthesis in the laboratory.

His work on functional materials began with the discovery of new classes of superconducting materials - superconductors transmit electricity without electrical resistance. In addition to this new class of superconductors, he has discovered new chemical reactions that access materials with control of structure at low temperatures that have recently allowed the research community to access the first non-copper based analogues of the high temperature superconductors. This has opened new paths to the transmission of electrical power without loss of energy. Materials also play a key role in information technology because they are used to store and process the information. Rosseinsky was the first to demonstrate a material that is both ferromagnetic and ferroelectric at room temperature, coupling the alignment of both electrical and magnetic dipoles – such multiferroic materials can reduce the energy required to read and write information. Rosseinsky has identified new classes of solar absorber based solely on non-toxic components, as well as introducing new families of lead-free piezoelectrics: piezoelectrics are used in actuators and sensors.

New energy technologies based on batteries and fuel cells require new materials. He identified new types of fuel cell cathode where distinct phases are cooperatively organised at the nanoscale to combine high performance with stability. He has developed new solid electrolytes for lithium batteries, and new approaches to both lithium and sodium ion battery cathodes. In heterogeneous catalysis, he has developed robotic approaches to accelerate the identification of catalysts to turn carbon dioxide into fuels and chemicals, key transformations for a sustainable society. He is well-known for his work on porous solids, a class of materials widely used in industrial catalysis and separation processes. Here he produced the first chiral microporous material, demonstrated new mechanisms for gas storage and created porous materials that display the induced fit and conformational selection responses of biological molecules.

In order to accelerate the realisation in the laboratory of such materials, Rosseinsky has worked with colleagues across physical and computer science to develop a suite of digital tools and workflows that harness artificial intelligence, machine learning and physics-based computation with automation. The aim of these digital methods is to enable the synthesis of outperforming energy materials not tied to those currently in materials databases, allowing us to harness the structural and compositional diversity offered by chemistry to access energy materials. This has enabled the *de novo* computationally guided laboratory synthesis of new materials with previously unknown structures, and the synthesis of new materials with very low thermal conductivities driven by a combination of structure prediction and machine learning. His team reported the inorganic material with the lowest thermal conductivity known by developing new chemistry involving the unusual presence of three different anions in the same compound, illustrating the coupling between digital methods and chemical exploration. Low thermal conductivity is key in heat management, for example in battery technology, thermoelectric waste heat harvesting and thermal barrier coatings for gas turbines. This reflects the societal benefit of generating distinctive structures with outstanding properties from the new chemistry opened by this methodology. Integrating these advances, he defined a collaborative AI approach that fuses human understanding with numerical ranking of candidate chemistries by machine learning to accelerate discovery of electrolytes for solid state batteries, further demonstrating how digital tools and workflows can afford materials for key application challenges. Most recently, he and colleagues reported an algorithm for both classical and quantum computers that guarantees to predict the structure of any crystalline material just based on knowledge of the atoms that make it up, transforming our ability to evaluate currently unexplored chemical space to identify candidate materials for application.