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Introduction to the special issue on energy materials

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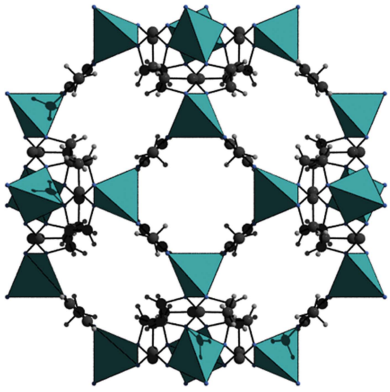
The relationship between structure and properties is one of the most important and pervasive paradigms in the physical sciences. It provides a means for understanding complex behaviour in materials at an atomistic level, and establishes a framework for the design of materials with specifically targeted properties. *Acta Crystallographica Section B* has a long tradition of publishing citation classics in the field of Materials Science, including seminal papers in bond valence analysis and the structural chemistry of perovskites, framework materials and ionic conductors. The recent change in the title of *Acta B* to include Structural Science, Crystal Engineering and Materials reflects not only the broad scope of the articles we publish, but also our ambition to attract new authors in these rapidly developing fields. An important component of the Editorial Board's strategy for encouraging this is to commission special issues devoted to key areas, and in this issue we focus on Energy Materials.

The need for secure, sustainable and affordable sources of energy is one of the greatest scientific challenges we currently face. The news is full of looming energy crises; the fossil fuels on which modern society has been built are becoming more difficult and more expensive to extract; nuclear power has failed to live up to the 'free energy' expectations of the 1950s; renewables such as wind power appear likely to remain relatively minor sources of energy for the foreseeable future.

The energy landscape evolves constantly as natural energy reserves are consumed and discovered, and as technological advances provide access to new alternative energy sources. Optimizing energy storage, conversion, distribution and utilization within the energy ecosystem is critical, not only to our energy security, but to economic stability and environmental stewardship. These energy needs drive widespread materials research. Materials are central to a wide range of energy technologies, from improved sensors for a more resilient electrical grid and higher power batteries for electric vehicles to selective capture materials that facilitate safe nuclear energy usage.

The area of molecular storage is highly relevant to many energy-related applications if one considers the move towards hydrogen as a 'clean' fuel and the need to capture, transport and release small molecules, as and when required for use. Related to the storage of fuels is the remediation of polluting gases, such as carbon dioxide and oxides of nitrogen, and this requires methods for the selective removal of undesirable species from complex mixtures in exhaust streams. Open-framework solids are one of the most heavily researched families of materials for these purposes, making use of internal porosity to absorb large amounts of guest molecules. Although such properties are long established for microporous zeolites the field is being revitalized presently with the discovery of metal–organic frameworks.

Crystallography often holds the key in establishing structure–property relationships in porous solids, allowing not only the structure of the framework to be determined, but also the location of guest molecules, permitting their interaction with the solid host to be rationalized. Several papers in this issue deal with such questions: for example, Chen *et al.* (2015) describe crystal structures of new framework solids prepared by 'superpolyhedral' building blocks that have desirable gas adsorption properties, while Chevreau *et al.* (2015) use powder neutron diffraction to understand the sorption properties of coordinaton polymers. Some considerable effort is needed to understand even the fundamentals of the physical properties of framework solids and Fletcher *et al.* (2015) describe a systematic approach to understanding framework flexibility using new data from a zeolite as an example. The emerging field of the effect of pressure on framework



materials, which can probe the mechanical properties as well as provide exhaustive information on pore accessibility and the potential energy landscape of the framework itself, is reviewed by McKellar & Moggach (2015). The structural chemistry of non-framework materials for hydrogen storage is discussed by Bennett *et al.* (2015) and by Cerný & Schouwink (2015), the latter delineating the structural relationship between metal borohydrides and oxides.

Batteries provide energy storage in personal electronics, electric and hybrid-electric vehicles, and for grid storage coupled to intermittent energy sources such as wind and solar power. Research in battery materials seeks to increase capacity, power, lifetimes, at reduced cost and with improved safety. However, understanding the factors which govern and limit battery performance is an immense characterization challenge. Device operation relies on coupled changes in structure, chemistry and electronic state from the atomic scale to the full device level. Accordingly, a wide variety of different crystallographic characterization tools are often employed to understand the function and failure in battery systems. This includes X-ray absorption spectroscopies, exemplified by Ashton *et al.* (2015) in probing the change in valence state as an electrode is charged and discharged, and by Reichardt *et al.* (2015) and Bianchini *et al.* (2015), who apply neutron and X-ray diffraction and pair distribution function analysis to probe the atomic structure. These papers illustrate the increasing use of *operando* experiments applied to study the dynamic processes of charging and discharging.

An important goal in the field of sustainable energy is the improvement in the efficiency of solar cells. The discovery of efficient photovoltaic cells based on lead iodides has sparked renewed interest in this class of materials in the context of solar cell technology, and the remarkable structural diversity arising from differing assemblies of lead-iodine anions is investigated by Weber *et al.* (2015). The role played by polymorphism of semiconductor materials for solar cell applications is explored by computational modelling of copper-based mixed metal oxides by Scanlon & Walsh (2015). The role and importance of disorder in determining the properties of energy materials is the theme addressed in several papers in this issue. The incommensurately modulated thermoelectric material manganese silicide is discussed by Akselrud *et al.*, 2015), while two papers by Wind *et al.* (2015) and Hori *et al.* (2015), applied to superionic conduction, focus on disorder in the form of commensurate modulation or non-stoichiometry. Total scattering analysis is applied to amorphous metal oxide films of interest as photoactive components of artificial leaf devices by Kwon *et al.* (2015).

This special issue demonstrates the central importance of crystallographic tools in the development of materials and technologies related to energy by probing the structure–function relationship to reveal the fundamental basis for device operation and failure. By exploring the structure and chemistry of energy materials, including *in situ* during operation or under conditions that lead to failure, performance limitations can be eliminated and thereby improve function in the next generation of materials and devices.

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