The Department of Chemistry, University of Massachusetts Amherst
presents

CLARE P. GREY

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Developing and Optimising Function of Li-ion and "beyond-Li" Batteries: New Magnetic Resonance and Diffraction Approaches

Tuesday, February 5, 2019
11:30 a.m.
Lederle Graduate Research Tower 1634
Refreshments at 11:00 a.m.

Five College
Chemistry Lecture Series

Five Colleges, Incorporated is a nonprofit educational consortium established in 1965 to promote the broad educational and cultural objectives of its member institutions, which include four private, liberal arts colleges and the Amherst campus of the state university. The consortium is an outgrowth of a highly successful collaboration in the 1950s among Amherst College, Mount Holyoke College, Smith College, and the University of Massachusetts Amherst, which resulted in the founding of a fifth institution, Hampshire College, in 1970.

Five Colleges promotes and administers long-term forms of cooperation that benefit faculty, students, and staff. These include:

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Their proximity to one another in the Connecticut River Valley of western Massachusetts favors *Five College* collaboration, as does their commitment to the liberal arts and to undergraduate education. *Five Colleges, Incorporated* is a longstanding member of the Association for Consortial Leadership (ACL), a national organization of consortia.

February 4 & 5, 2019
Challenges in Designing New Batteries and Supercapacitors for a Low Carbon Economy

February 4th
Cleveland Hall L1
Mount Holyoke College, 4:30 p.m.

February 5th
Ford Hall, Room 240
Smith College, 5:00 p.m.

Clare Grey

Clare P. Grey, FRS is the Geoffrey Moorhouse-Gibson Professor of Chemistry at Cambridge University and a Fellow of Pembroke College Cambridge. She holds a Royal Society Professorship. She received a BA and D. Phil. (1991) in Chemistry from the University of Oxford. After post-doctoral fellowships in the Netherlands and at DuPont CR&D in Wilmington, DE, joined the faculty at Stony Brook University (SBU) as an Assistant (1994), Associate (1997) and then Full Professor (2001-2015). She moved to Cambridge in 2009, maintaining an adjunct position at SBU. She was the director of the Northeastern Chemical Energy Storage Center, a Department of Energy, Energy Frontier Research Center (2009-2010) and Associate director (2011-2014). She is currently the director of the EPSRC Centre for Advanced Materials for Integrated Energy Systems (CAM-IES). Her recent honours and awards include the 2011 Royal Society Kavli Lecture and Medal for work relating to the Environment/Energy, Honorary PhD Degrees from the Universities of Orleans (2012) and Lancaster (2013), the Gunther Laukien Award from the Experimental NMR Conference (2013), the Research Award from the International Battery Association (2013), the Royal Society Davy Award (2014), the Arfvedson-Schlenk-Preis from the German Chemical Society (2015), the Société Chimique de France, French-British Prize (2017) and the Solid State Ionics Galvani-Nernst-Wagner Mid-Career Award (2017). She is a foreign member of the American Academy of Arts and Sciences (2017) and a Fellow of the Electrochemical Society (2017). Her current research interests include the use of solid state NMR and diffraction-based methods to determine structure-function relationships in materials for energy storage (batteries and supercapacitors), conversion (fuel cells) and carbon capture.

ABSTRACT: *The development of light, long-lasting rechargeable batteries (and the invention of the lithium-ion battery, now over 25 years ago) has been an integral part of the portable electronics revolution. This revolution has transformed the way in which we communicate and transfer and access data globally. Rechargeable batteries are now playing an increasingly important role in transport and grid applications, but the introduction of these devices comes with different sets of challenges. New technologies are being investigated, such as those using sodium and magnesium ions instead of lithium, and the flow of materials in an out of the electrochemical cell (in redox flow batteries). Importantly, fundamental science is key to producing non-incremental advances and to develop new strategies for energy storage and conversion.*

The first part of this talk will focus on our work on the development of methods that allow devices to be probed while they are operating (i.e., in-situ). This allows, for example, the transformations of the various cell components to be followed under realistic conditions without having to disassemble and take apart the cell. To this end, the application of new in and ex-situ Nuclear Magnetic Resonance (NMR), magnetic resonance imaging (MRI) and X-ray diffraction approaches to correlate structure and dynamics with function in lithium- and sodium-ion batteries and supercapacitors will be described. The in-situ approach allows processes to be captured, which are very difficult to detect directly by ex-situ methods. For example, we can detect side reactions involving the electrolyte and the electrode materials, sorption processes at the electrolyte-electrode interface, and processes that occur during extremely fast charging and discharging. Complementary Ex-situ investigations allow more detailed structural studies to be performed, to correlate local and long-range structure with performance. To illustrate, we have used NMR, theory and pair distribution function (PDF) analysis methods, to determine the local and longer range structures of a series of amorphous and disordered Li and Na anode structures, including C, Sn, Ge, Si and P. Both thermodynamic and metastable phases are identified via theoretical (DFT) approaches and compared with NMR, PDF and (in situ) diffraction measurements, the materials often transforming via metastable structures. Finally, many of the battery electrode materials are paramagnetic and their study has involved the development of new experimental (NMR) and theoretical approaches to acquire and interpret spectra. Recent studies to correlate lithium hyperfine shifts with local structure and to probe dynamics will be described.