

$x\text{Sm}_x\text{Se}_3$ system. Comparisons will be made with quantitative chemical analyses obtained through the use of inductively coupled plasma (ICP) analyses.

Finally, the compound $\text{Ba}_4\text{Fe}_2\text{I}_5\text{S}_4$ will be used to illustrate the structural challenges posed by the unexpected in solid-state syntheses.

Keywords: metal chalcogenides, chemical crystallography, physical properties structure relationships

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The Importance of Structure in the Design of Lithium Battery Materials

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Since 1990, rechargeable lithium batteries have made a huge impact in powering consumer electronic devices such as cell phones and laptop computers [1]. The need for new insertion electrode structures that will provide additional energy, power and a superior cycle life to satisfy the increasing demands for reliable and safe high-energy/high power batteries by the transportation, medical, space, and defense sectors will ensure that lithium battery research will continue for many more years to come. This presentation will review the progress that has been made over the past 15 years and it will highlight the critical role that structure plays in the design and operation of lithium battery electrodes. Recent advances that have been made in designing two-component, structurally-integrated materials to achieve performance objectives will be discussed [2, 3]. The presentation will be made in the context of the advantages and limitations of other battery systems.

[1] Tarascon J.M., Armand M., *Nature*, 2001, **414**, 359. [2] Kim J-S., Johnson C. S., Vaughney J. T., Thackeray M. M., Hackney S. A., Yoon W., Grey C. P., *Chem Mater.*, 2004, **16**, 1996. [3] Thackeray M. M., Johnson C. S., Vaughney J. T., Li N., Hackney S. A., *J. Mater. Chem.*, 2005, *in press*.

Keywords: lithium battery, insertion electrode, structure

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Pore-Forming Toxins

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Pore-forming protein toxins (PFTs) are one of Nature's most potent biological weapons. They are produced by a variety of living organisms, particularly bacteria, certain insects, poisonous reptiles and stinging marine invertebrates. As offensive weapons these toxins can aid digestion or degeneration of the host whilst as defensive weapons they can protect by killing invaders. Of the more than 300 protein toxins characterized to date, at least a third act by disrupting membranes. In order for these water-soluble proteins to insert into membranes they must undergo a series of conformational changes to expose or generate new hydrophobic surfaces that can penetrate the core of cell membranes.

We have determined the crystal structures of a number of microbial pore-forming toxins. Although the structures are quite different they reveal common features that have been implicated in the mechanism of membrane insertion into cells. Two of these toxins belong to the family of cholesterol-dependent cytolysins (CDCs). CDCs exhibit a number of unique features amongst pore-forming toxins including an absolute dependence on the presence of cholesterol-rich membranes for their activity and the formation of very large oligomeric transmembrane pores greater than 15 nm in diameter. The crystal structures of these toxins suggest how they recognise cholesterol and provide the basis, together with available cryoelectron microscopy data, for modelling their pores.

Keywords: toxins, channel proteins, membrane associated proteins

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Pressure Induced Complexity in the Elements

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At ambient pressure, the metallic elements typically adopt high-symmetry crystal structures such as bcc, fcc and hcp. However, on compression, many of these simple structures undergo a series of structural transitions to phases characterised by considerable structural complexity, and it is only with recent advances in high-pressure single-crystal and powder-diffraction techniques that many of them have been determined. In the group 1, 2, and 15 elements, we have found a number of incommensurate "hotel" structures comprising interpenetrating host and guest structures [1]; transitions between these composite structures [2]; modulations of the host and guest structures; a transition to a composite structure with a "liquid" guest component [3]; and a number of surprisingly complex commensurate structures. And in the group 16 elements, we have found a number of incommensurately modulated structures that are stable over a remarkably wide range of pressures and temperatures [4]. I will review all the recent results on these "simple" metals, and discuss possible explanations for the existence of this complexity.

[1] McMahon M. I., Degtyareva O., Nelves R. J., *Phys. Rev. Lett.*, 2003, **85**, 4896. [2] Nelves R. J., Allan D. R., McMahon M. I., Belmonte S. A., *Phys. Rev. Lett.*, 1999, **83**, 4081. [3] McMahon M. I., Nelves R. J., *Phys. Rev. Lett.*, 2004, **93**, 055501. [4] Hejny C., McMahon M. I., *Phys. Rev. Lett.*, 2003, **91**, 215502.

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Electrostatic and Related Properties from Accurate Charge Density Analyses

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Properties of atoms and molecules in crystals are now commonly extracted from a combination of X-ray diffraction experiments and theoretical results from a variety of approaches. Modern quantitative charge density studies typically involve use of CCDs and/or synchrotrons, T below 120 K and frequently nearer 10 K, careful data reduction and correction for systematic effects, and detailed modelling of atomic motion. Multipole refinement yields topological properties of the electron density in almost all studies, while valuable electrostatic properties are seldom reported. Yet there is a wealth of such properties accessible from the X-ray experiment: electrostatic potential, electric field and field gradient, atomic charges, electric moments of molecules in the crystal, and even intermolecular interaction energies.

If we accept that "theory is a good thing but a good experiment is forever" [1], we must ask: Are we maximizing the information that can be obtained from charge density data sets? If not, why not, and how might this be redressed? This presentation will seek answers to these questions from a discussion including results from a selection of recent studies. Limitations of some of the common approaches will be highlighted, and some solutions will be proposed, along with comments on related properties that might be explored.

[1] Kapitzka P.L., *Experiment, Theory, Practice*, (D. Reidel, Boston), 1980, 160.

Keywords: charge density studies, electron density studies, electrostatic properties

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Structural and Functional Studies of Large Macromolecular Assemblies

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The main goal of the research in my laboratory is to study structure and function of large macromolecular assemblies involved in central cellular processes. Although most of our work focuses on