Recent advances and the exciting potential in a range of these areas will be discussed, including studies of proton migration, investigations of thermal parameter trends, hydrogen atom disorder, polymorphism, weak hydrogen bonded interactions and studies of molecular materials under high pressure.
The potential for future developments in both science and instrumentation of relevance to neutron diffraction studies of molecular structure will also be discussed.

KN14

From Small Moleculaes to Extended Structures Leonard J. Barbour, *Department of Chemistry, University of Stellenbosch, South Africa.* E-mail: ljb@sun.ac.za

Nature embraces the principles of supramolecular chemistry by exploiting non-covalent interactions in a multitude of ways to facilitate all biological processes. The facile assembly of complex synthetic systems in both solution and the solid state is becoming increasingly feasible and there is significant interest in the encapsulation of chemical space. This often requires that known systems be modeled, explored and fine-tuned in order to develop further systems of even higher complexity. Examples include the construction of globular or spheroidal self-assembled molecular capsules, which have potential applications as drug delivery agents, van der Waals catalysts, nano-reactors and mimics of biological systems. Spheroidal assemblies are generally highly symmetrical and frequently assume the shapes of the Platonic or Archimedean solids. For example, the cowpea chloritic mottle virus is comprised of 180 identical protein subunits assembled into an icosahedron. Under pH control the overall conformation of the viron changes, giving rise to pores in the outer shell, thus allowing the passage of molecular material between the interior of the viral cavity and its environment. Although gaining analogous control over the size, conformation and composition of synthetic systems is a formidable challenge, advances have been made in influencing both the volume and composition of enclosed chemical space within the shells of non-covalent capsules assembled mostly by means of hydrogen bonding. These and other extended assemblies will be discussed.

KN15

***In situ* examination of Li-ion battery materials** Helmut Ehrenberg[a,b], Natalya N. Bramnik[b], Kristian Nikolowski[a,b] [a]*Institute for Complex Materials, IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany* [b]*Institute for Materials Science, Darmstadt University of Technology,Petersenstr. 23, D-64287 Darmstadt, Germany.* E-mail: h.ehrenberg@ifw-dresden.de

Keywords: Lithium ion batteries, positive-electrode materials, *in situ* diffraction study

Electrode materials in rechargeable lithium ion batteries undergo significant structural changes during charging and discharging, i.e. lithium extraction and insertion. Both the local structural changes due to the accompanied redox-reaction and the global changes in volume for different charge states are of primary importance for the electrochemical performance of such materials. An investigation of the relationship between crystal structure and electrochemical properties requires *in situ* studies under real operation conditions, because the disassembling of the battery will most probably affect the electrode materials and falsify the structural characterisation. We have developed dedicated test cells, which allow *in situ* studies in transmission geometry up to at least 150 charge-discharge cycles [1], so that correlations with the capacity loss due to limited cycle stability become accessible.
In this contribution we report on structural studies on the most relevant positive electrode materials for lithium ion batteries and the role of the underlying crystal structures for the resulting electrochemical properties. In addition to induced phase transitions during conditioning the importance of microstructural aspects for degradation phenomena will be emphasized.
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[1] Nikolowski K., Baehtz C., Bramnik N. N., Ehrenberg H., *J. Appl. Cryst.*, 2005, 38, 851-853.

KN16

Multiprotein machines for gene transcription Patrick Cramer *Gene Center Munich, Ludwig-Maximilians-Universität München, Munich, Germany.*
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Keywords: Multiprotein complex, transcription, X-ray crystallography

The current state of our structure-function analysis of the mRNA gene transcription cycle will be discussed. The crystallographic structures of the complete 12-subunit RNA polymerase II in free form and with bound DNA and RNA have been determined as atomic models. The structure of the complete Pol II elongation complex bound by the transcript cleavage factor TFIIS explained how Pol II uses a single tunable active site for both RNA synthesis and RNA cleavage. Three structures of complexes of CTD-interacting proteins provided insights into the coupling of transcription elongation to mRNA processing and histone methylation, and into Pol II recycling. The first structure of a Pol II complex with an RNA inhibitor and the first atomic structures of subcomplexes of the Mediator of transcriptional regulation provided insights into gene regulation. A set of new structures of Pol II bound to damaged DNA together with complementary functional assays revealed unexpected mechanisms of lesion recognition during transcription-coupled DNA repair. Unpublished data show that we can use hybrid methods to obtain new insights into the structure and function of the two other RNA polymerases, Pol I and Pol III.

KN17

Reciprocal space phasing methods for reconstructed surfaces Jordi Rius, *Institut de Ciència de Materials de Barcelona (CSIC), Campus de la UAB, Catalunya, Spain.*
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Keywords: GIXRD, phasing methods, surface diffraction

In the last years the application of GIXRD to the study of reconstructed surfaces has experienced considerable progress. The principal reasons have been the easier access to 3rd generation synchrotron sources, the increasing computer power but also the development of new methods for the solution of reconstructed surfaces.