experimental and theoretical levels.

The experimental data accumulated to date on the synthesis and characterization of silicates mesoporous materials strongly support the view that a good theoretical model will be most suitably grounded on the aggregation colloids chemistry and on the lyotropic liquid crystal physico-chemistry. Some aspects, specific to the unique ability of silicates to polymerize must also be included to get a coherent picture. A short review of the backgrounds in these fields, with a special emphasis on X-ray diffraction techniques, will be made.

Then, experimental data illustrating the differences and similarities existing between the 'standard' lyotropics liquid crystals and the silicatropic liquid crystals will be presented. This comparison helps to identify the leading forces governing the formation of the silicatropic mesophases and their subsequent polymerization. In turn this allows a model to be presented which is consistent with the behavior of the silicate-surfactant supramolecular assemblies observed so far. The proposed model provides insight into how the various synthesis conditions favor a particular morphology and also suggests possible synthesis modifications to enhance the quality of the final material.

Finally, recent diffraction experiments revealing various phase transitions occurring during the synthesis of the mesoporous material will be presented. The occurrence of these phases transitions will be discussed within the frame of the above proposed model.

As a conclusion, several directions for future investigations will be outlined with their potential consequences for the development of this rapidly growing research field.

KY.NT.21 GROWTH, CHARACTERIZATIONS & APPLICATIONS OF DIAMOND FILMS. Pieter Bennema

KY.NT.22 PROTEIN STRUCTURES: THEIR VALIDATION FOLD CLASSIFICATION AND INTERACTIONS. Janet M. Thornton[1,2], E.G. Hutchinson[1], S. Jones[1], R.A. Laskowski[1,2], M. W. MacArthur[1], A. Michie[1] and C.M. Orengo[1], [1]Department of Biochemistry and Molecular Biology, University College, Gower Street, London WC1E 6BT, [2] Department of Crystallography, Birkbeck College, Malet Street, London WC1E 7HX

As the number of known protein structures rises rapidly, we begin to appreciate the extent of the universe of protein folds. For each new structure apart from its unique biological interest, it is essential to validate the co-ordinates, to describe the structure in terms of its relationship to other known structures and their functions, and to study the interactions made by the protein with other biomolecules. Since structures are often solved very rapidly it has become essential to develop approaches and software tools which facilitate automated validation, analysis and classification of the structure for the crystallographer. These tools are valuable for users of the databank .

In this presentation, three different aspects of structural analysis will be considered. First, methods for validating structures, based on current knowledge derived from known structures will be discussed. These methods complement the critical measure of agreement between the model and X-ray data. Recent results derived from very high resolution structures will be presented. Secondly, as the size of the database grows it becomes more difficult to know whether a structure is novel or has been seen before. Our hierarchical description of protein structure in terms of Class, Architecture, topology and homologous superfamily (CATH) will be described. Lastly, novel approaches to identifying active sites and recognition patches on the surface of a protein will be discussed.

Information available at http://www.biochem.ucl.ac.uk/bsm

KY.NT.23 DIRECT METHODS IN REAL AND RECIPROCAL SPACE. George M. Sheldrick, Universität Göttingen, Germany

Conventional direct methods that use probability relations to determine the phases of a limited number of reflections are computationally extremely efficient for small structures, but the chances of success decrease sharply as the number of independent atoms increases above about 200. They also require fairly complete data to atomic resolution. It appears that the size barrier has at last been broken by methods that iterate between real and reciprocal space, pioneered by the 'Shake and Bake' program developed by the Buffalo group (Miller et al., 1993). Given a powerful enough computer, much larger structures can be solved than were possible with pure reciprocal space direct methods. The success rate can be improved if slightly better than random starting phases are available, e.g. from automated Patterson interpretation (Sheldrick & Gould, 1995). Such a Patterson-based structure expansion enabled the ab initio solution of a small metalloprotein with about 840 non-hydrogen atoms in the asymmetric unit (Frazao et al., 1995). However these methods still require data to atomic resolution, which in practice means about 1.2 Å.

The next breakthrough will probably be the more active use of general structural knowledge in the real-space part of these procedures, rather than simply peak picking; it is possible that this will lead to a relaxation of the atomic resolution requirement. This talk will review recent progress towards the ab initio solution of both small-moiety and macromolecular structures.

C. Frazao, C.M. Soares, M.A. Carrondo, E. Pohl, Z. Dauter, K.S. Wilson, M. Hervas, J.A. Navarro, M.A. De la Rosa & G.M. Sheldrick (1995). *Structure* 3, 1159-1169.

R. Miller, G.T. DeTitta, R. Jones, D.A. Langs, C.M. Weeks & H. Hauptman (1993). *Science* 259, 1430-1433.

G.M. Sheldrick & R.O. Gould (1995). Acta Cryst. B51, 423-431.

KY.NT.24 NEUTRON DIFFRACTION STUDIES OF COORDINATION AND ORGANOMETALLIC COMPOUNDS. Thomas F. Koetzle, Chemistry Department, Brookhaven National Laboratory, P.O. Box 5000, Upton, NY 11973-5000 USA

In the 50 years since Shull and Wollan's pioneering experiments at Oak Ridge National Laboratory, neutron diffraction has been used to attack a wide range of structural problems in inorganic and organometallic chemistry. These studies exploit the unique properties of neutrons that make them a powerful probe and complement to x rays in crystallographic research. Neutrons are highly sensitive to hydrogen and light atoms in general, have the ability to reveal nuclear positions and mean displacements without bias from the effects of the electron distribution, can detect isotopic substitutions, and are sensitive probes of magnetism.

This lecture will concentrate on single-crystal neutron diffraction, and will illustrate the field with examples taken from work at both reactor and spallation neutron sources. Topics discussed will include structures of metal hydrogen compounds, use of deuterium labelling to investigate reaction mechanisms, structures of ice and gas clathrate hydrates, and studies of spin-density distributions in open-shell systems.

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