

research questions, collaborate with those having greater expertise, utilize crystallographic results as the basis for or validation of their own work, and critically review published structures or those being submitted for publication. Opportunities, challenges and pedagogical implications presented by these policies and cyber instruction will be discussed.

Keywords: teaching, policy, cyberinfrastructure

### MS.11.4

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#### Use of images from neolithic art, clip art, digital cameras, and MATLAB® in teaching crystallography

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Images illustrating symmetry are valuable in the teaching of crystallography. Unusual two-dimensional wall-paper patterns from Neolithic art collected by Prof. Slavik Jablan will be shown. Amazing illustrations of two-dimensional point groups and space groups have been constructed by students using clip art with programs such as Microsoft Paint. Digital cameras can be used to collect imaginative examples of crystallographic interest such as reflections in ponds, spiral-staircase screws, and footprints-in-the-sand glide planes. Advanced computer languages like MATLAB® can be used to create parametric figures such as spirals, seashells, and butterflies (T.H. Fay *Amer. Mat. Mon.* 96, 443, 1989) which then can be inserted in space groups. Illustrations will show teaching examples and student exercises, many from *Foundations of Crystallography with Computer Application* by Maureen M. Julian, CRC press 2008.

Keywords: crystallographic education, computer-aided instruction, symmetry

### MS.11.5

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#### Teaching crystallography: Approaches for non-crystallographers and non-native speakers in Asia

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The teaching of crystallography, as a cross-disciplinary science, is required in a variety of subject areas and at different academic levels. Some of the approaches and curricula of crystallography developed at a technological university in Asia, and given at the undergraduate or introductory level in Solid State Chemistry and Materials Science and Engineering, as well as at the post-graduate level in a one-semester course on Chemical X-ray Crystallography are reviewed. The needs of non-crystallographers, and even non-native speakers, can pose additional challenges for successful teaching and learning outcomes. The use of visual constructs and in-class exercises to develop understanding is thus emphasized. The fundamentals of crystallographic symmetry and both powder and single crystal diffraction can be tackled via case studies of increasing complexity, starting from 2D patterns and progressing through simple 3D inorganic structures to complex organic or protein molecular packing arrangements. At more advanced level the conceptual background seems best augmented by combination with experimental practice.

The Asian region has some of the most disparate levels of educational and scientific resources in the world. Many sizeable countries within it do not have even one single crystal X-ray diffractometer. A case is presented for the need of a workshop-based crystallographic school, with hands-on access to modern instrumentation, to promote and sustain crystallography in the less developed parts of the region.

Keywords: crystallographic teaching, inorganic and organic crystal structures, materials engineering teaching programme

### MS.12.1

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#### X-ray scattering studies of liquid-crystalline suspensions of anisotropic mineral nanoparticles

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Mineral liquid crystals are colloidal suspensions of anisotropic (disc-like or rod-like) mineral nanoparticles in a solvent, usually water. These suspensions form various types of liquid-crystalline nematic, lamellar, or columnar phases, depending on the particle anisotropy and concentration. Such phases combine long-range orientational order of the particles with either short-range positional order or long-range positional order in 1 or 2 dimensions. X-ray scattering is a very well suited technique to study these properties because it gives direct access to the nematic order parameter, and to the dimensionality and symmetry of the positional order. This will be illustrated by various examples: Suspensions of goethite (FeOOH) nanorods provide a very convenient system because it displays all the above-mentioned phases [1,2], sometimes coexisting in a single sample [3]. Besides, suspensions of natural clays will be used to describe the case of disc-like particles [4,5]. Moreover, if time allows, I will also show how the dynamic properties of nematic suspensions of rod-like nanoparticles can be probed by the rather new technique of X-ray photon correlation spectroscopy (XPCS).

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Keywords: liquid crystals, colloids, small-angle scattering

### MS.12.2

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#### Crystallography of 2D and 3D structures in liquid crystal amphiphiles and nanocomposites

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A combination of X-ray diffraction methods was used to study thermotropic phases of three groups of liquid crystalline materials. The different experimental and analysis techniques used will be illustrated on selected examples. Firstly, a wide range of T-shaped, X-shaped and  $\pi$ -shaped amphiphiles with three or four incompatible moieties were studied. A range of novel phases with 2D and 3D

order on the 2-20 nm scale were discovered. Secondly, a complex cubic phase of some polycatenar LCs (rod-like molecules with more than one appended terminal chain) is investigated. Thirdly, packing of gold nanoparticles coated with nematogens is studied. Powder, single domain and fibre patterns are used, as appropriate, with GISAXS proving particularly useful. Electron density reconstruction is used routinely, but to help solve the phase problem a number of methods are used, including different variants of isomorphous replacement, model building and refinement, and supporting neutron scattering experiments. The main conclusion is that, with the ever increasing complexity of liquid crystal phases, the simple comparison of spacings and molecular dimensions as a method of structural characterization, often used in the past, is increasingly becoming a thing of the past.

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Keywords: liquid crystals, GISAXS, cubic phases

## MS.12.3

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### Molecular aggregation structure of exotic liquid crystals formed by thermotropic mesogen BABH(n)

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1,2-Bis(4'-n-alkoxybenzoyl)hydrazines [BABH(n), n: the number of C atoms in an alkoxy chain] exhibit micro phase separated liquid crystalline phases: smectic C (lamellar) and two bicontinuous types of cubic phases (Ia3d & Im3m). According to Babinet's principle, reflection intensities do not give any information concerning the electron density, and consequently, the location of molecules. To locate molecules in complex structures, the authors utilized the chain length (n) dependence. For the Ia3d phase, widely observed in lyotropics and block copolymers, it is deduced that Gyroid, a triply periodic minimal surface (TPMS), is formed by the terminal methyl groups while the molecular cores aggregate as rods. This structure remains in  $3 < n < 23$ , in contrast to simple continuum theories of micro phase separation, which predict the interchange of roles of two components at both sides of the lamellar phase region appearing around the equivolume composition. For the Im3m phase ( $12 < n < 17$ ) that is observed only for low-molecular weight thermotropics, MEM analyses were systematically performed as the similar analysis to the Ia3d phase failed. The MEM formula was modified to use only their magnitude for reflections other than two main ones. The n dependence of the MEM results successfully solved the phase problem while making the theoretical consideration on the phase stability. The solution revealed that the molecular cores form a spreading jungle gym having three-fold junctions and spherical shells. The rods of the jungle gym are nearly on a TPMS (P surface). This structure of the Im3m phase clearly has similarities with both of the Ia3d phase and the lamellar phase: Spreading jungle gym with three-fold junctions and sheet-like aggregate (though closed on a sphere).

Keywords: liquid-crystal structures, maximum-entropy method, minimal surface

## MS.12.4

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### Mesophase semiconductors: Design for 3D-mesophases with effective paths for electronic charge hopping

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Liquid Crystalline Semiconductors are now evolved into Mesophase Semiconductors because of the importance of the highly ordered structure of mesophase [1]. On the other hand, Organic Electronics is a most interesting category of researches on organic condensed matter in terms of polymer-based thin film electronic devices and more efficient design strategies for the molecules are required. Recent studies on calamitic liquid crystalline systems have insisted the better situation to obtain the faster mobility of charged carriers does not meet ordinary and typical liquid crystalline phases such as nematic and smectic A phases and the more highly ordered systems do have an advantage in the mobility improvement. We recently reported that a mesogenic 8TNAT8 (an alkylated dithienyl naphthalene) showing a highly ordered mesophase with a 3D lattice have a fast carrier mobility in the order of  $10^{-1}$ - $10^{-2}$  cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup> in the mesophase where the molecules align just like a smectic layered phase. The application of this compound to a field effect transistor (FET) exhibits the comparable mobility (0.14 cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup>) at room temperature (crystalline solid) [2]. In this work, the 3D-mesophase structure was studied by powder X-ray diffraction (XRD) with a dilatometry technique and by single crystal XRD of the room temperature crystal. It was found that the room temperature crystal and the mesophase one are so similar to each.

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Keywords: organic electronics, liquid crystalline semiconductor, charge hopping path

## MS.12.5

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### Functional nanostructured liquid-crystalline assemblies

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Soft materials are molecular-based materials such as polymers, liquid crystals, and colloids. They are becoming important as functional materials because of their dynamic nature. Although soft materials are not as highly durable as hard materials such as metals and ceramics, they can respond to stimuli and environment. The introduction of molecular order into soft materials induces new dynamic functions.