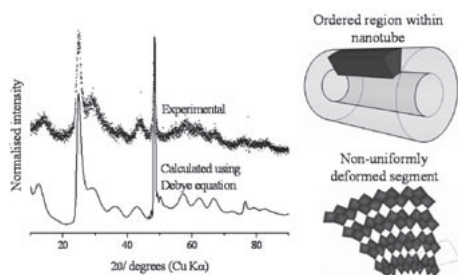


continuous increase in the interatomic distances extending radially outwards across the tube wall. The distances in the outer half of the tube are greater than those in the ideal structure, resulting in wider bottlenecks for  $\text{Li}^+$  ion transport, consistent with a higher rate of  $\text{Li}^+$  intercalation, and with the greater accessibility of  $\text{Li}^+$  sites, consistent with a higher maximum  $\text{Li}$  composition



Keywords: powder diffraction techniques, nanotubes, structure-properties relationships

### MS.32.4

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#### The application of a molecular replacement approach to the refinement of a copper nanoball complex

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The reaction of equimolar amounts of  $\text{Cu}(\text{NO}_3)$  and bdc-5-OH (benzene-1,3-dicarboxylate-5-hydroxy) is an example of a one-step synthetic method which may be used to generate nanoscale molecules via self-assembly. In this case, the discrete structures, termed 'nanoballs' are molecular versions of faceted polyhedra, namely small rhombihexahedra. The structural characterization of specific nanoball complexes,  $[\text{Cu}_2(\text{bdc-5-OH})_2\text{L}_2]_{12}$  (where L is a dimethyl sulfoxide, methanol or water ligand), via single crystal x-ray diffraction is very difficult. In many respects, the diffraction patterns obtained from these large metal-organic molecules resemble those obtained from protein crystals, largely due to disordered solvent molecules inside the nanoballs and between the nanoballs. We have utilized an approach similar to isomorphous replacement to refine the structure of  $[\text{Cu}_2(\text{bdc-5-OH})_2(\text{H}_2\text{O})_2]_{12}$  (1) from 1.4 Å data. An idealized small rhombihexahedron structure based upon the previously-determined  $[\text{Cu}_2(\text{bdc-5-OH})_2(\text{DMSO})(\text{MeOH})]_{12}$  (2) structure, was used to generate a 432-atom rigid body unit (with axially coordinated solvent ligands removed). The orthogonal Angstrom coordinates for this idealized unit were then imported into SHELXTL, using the FRAG instruction. This fragment was fit to the 48 Cu atoms for two independent molecules in structure 1, resulting in the generation of fractional coordinates for all of the nanoball atoms. Complex 1 crystallizes in the space group  $P2_1/n$  with  $a = 47.993(2)$  Å,  $b = 27.763(1)$  Å,  $c = 48.131(2)$  Å,  $\beta = 110.341(2)^\circ$ , volume =  $25095(1)$  Å<sup>3</sup>, with  $Z = 2$ . The Cu atoms were refined anisotropically and all other non-hydrogen atoms were refined isotropically to yield  $RI = 13.77\%$  for 13551 observed reflections and 1577 parameters.

Keywords: refinement problematic structures, SHELX, isomorphous replacement

### MS.32.5

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#### Coherent diffractive imaging of nanostructures at synchrotron and FEL sources

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Coherent X-ray Diffractive Imaging (CXDI) is a new microscopy technique that has potentiality to produce images up to diffraction limited resolution at x-ray wavelengths. The basic principles of the technique will be presented in this talk. A number of applications for imaging the shape and strain fields of the nanometer size crystals will be presented as well. It will be demonstrated how a few nanometer resolution can be achieved if a large number of identical samples are illuminated coherently. In the end recent results of CXDI at FLASH Facility at Hamburg will be given.

Keywords: coherent diffractive imaging, phase retrieval, nanosamples

### MS.33.1

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#### New liquid structures of alkali metals under pressure predicted from first principles theory

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We present results from *ab initio* calculations that predict a series of electronic and structural transitions in alkali liquids under pressure. The transitions are initially driven Peierls distortions in the local order of the liquids, followed at higher pressure by electron core overlap effects. In the case of Li, weakly bound tetrahedral clusters are found at pressures above 150 GPa. Similarities and differences between the phase diagrams of Li, Na and K are studied. We establish correlations between the solid and liquid phases of these elements, on the basis of which we predict their melting properties and provide evidence for the low-temperature crystalline phases likely to be found at extreme pressures.

Keywords: high-pressure physics, *ab initio* calculations, liquid structure

### MS.33.2

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#### Total scattering studies of pressure induced amorphization

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Solid state amorphization is a widely studied effect, recently highlighted in the interpretation of the structural process underlying rewritable digital versatile discs [1]. Pressure-induced amorphization (PIA) falls within this field and is typified by the behaviour of  $\text{ZrW}_2\text{O}_8$ . Indeed, the mechanism for amorphization in this system