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Keywords: copper compounds-1, biomimetics-2, catalyst structure -3

FA4-MS31-P04

Defect Engineering in Colloidal Photonic Crystals.

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Imaging of lattice defects in crystalline materials has captured the attention of the scientific community for many decades. Because the size of typical defects is of the order of the lattice period of a crystal, techniques to image stacking faults, dislocations and vacancies have never been able to resolve their structure down to the core level. By crystallizing micron-sized colloidal particles into close-packed structures, we are now able to study crystal structures and defects in real and reciprocal space. We use synchrotron microradian X-ray diffraction to image the average crystal structure over large crystalline areas. Through confocal microscopy, we also have access to the local crystal structure on a single particle level. The combination of these techniques enables us to identify the global crystal structure and explain it through the presence of local defects. Using this approach, we have identified a large concentration of intrinsic stacking faults in colloidal crystals that were previously thought to be pure face-centred cubic in structure. Through confocal microscopy we found Lomer-Cottrell dislocations to be responsible for the nucleation of these stacking faults. Exploiting this growth mechanism, we were able to selectively grow stacking faults into colloidal crystals by sedimentation onto a structured template containing a 2D projection of a Lomer-Cottrell dislocation. This is of interest for the applicability of colloidal crystals as photonic materials.

Keywords: defects, colloids, photonic crystals

FA4-MS31-P05

Magnetic Exchange Interactions through H-bonds in Copper(II) Carboxylates.

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Hydrogen bonds and coordination bonds are used as interesting tools for inorganic crystal engineering to build up building blocks that possess their application in supramolecular structures [1]. Some copper(II) complexes, as examples, have shown that the intermolecular hydrogen bonds can modified their magnetic properties [2]. Similar system of hydrogen bonds have been found in some supramolecular isomers [3] of the other copper(II) carboxylate complexes. We have recently published dinuclear complex $[Cu(\mu\text{-nia})(5\text{-MeSal})_2(H_2O)]_2$ (nia = nicotinamide, 5-MeSal = 5-methoxysalicylate anions) [4] and mononuclear complex $[Cu(nia)(3\text{-}NO_2Bz)_2(H_2O)_2]$ ($3\text{-}NO_2Bz$ = 3-nitrobenzoate anion) [5], which exhibit similar magnetic properties. Very similar magnetic properties of mononuclear and binuclear complexes could be explained by the presence of very similar supramolecular synthons that are pathway for the magnetic exchange interactions. The hydrogen bonds, described by supramolecular synthons, formed by coordinated water molecule and two carboxylatogroups on each copper atom could create supramolecular dimers of two mononuclear complex molecules [4] and supramolecular chains of dinuclear complex molecules [5]. In this report we present series of 1-D coordination polymers of general formula $[Cu(\mu\text{-dena})(RCO_2)_2(H_2O)]_n$ (RCO_2 are substituted benzoate or salicylate anions, dena = N,N-diethylnicotinamide) with similar magnetic properties, that are explained as a consequence of the supramolecular synthons allowing to create two dimensional layer structures based on the 1-D coordination polymers bonded by hydrogen bonds. This could be given as the proof, that the hydrogen bonds described above are the main path for observed magnetic exchange and for that reason the simmilarity in magnetic properties (maximum of susceptibility at similar temperature and the value of antiferromagnetic interactions $2J$) are observed in all complexes, despite they are of different crystal structures, and different dimensionality (monomeric, dimeric, or polymeric).

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Keywords: crystal structure, hydrogen bonds, magnetic exchange interactions

FA4-MS31-P06

Cocrystals of flucytosine: Models for drug-receptor interactions.

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Flucytosine (5-fluorocytosine) is a systemic antifungal drug. It is intrafungally converted into 5-fluorouracil and inhibits RNA and DNA synthesis [1]. Furthermore, it has a novel application as a prodrug active against liver tumours [2]. The interaction between flucytosine and its receptor, as well as the base pairing, can be imitated by hydrogen-bonded complexes [3]. In order to examine these interactions we cocrystallized flucytosine together with several model compounds containing complementary functional groups and studied the preferred conformations adopted by the model compounds.
Since the cocrystallization of supramolecular complexes is not a straightforward procedure, we have developed a concept for designing these structures. After selection of model compounds, we calculate the structures and energies of a multitude of alignments ("constellations") by our force-field program MOMO [4]. Various analytical tools (especially IR spectroscopy and powder diffraction) are used to identify the