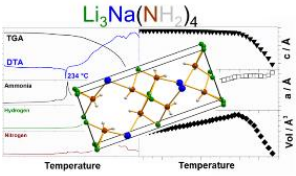
Center for Materials Crystallography: Highlights in 2016

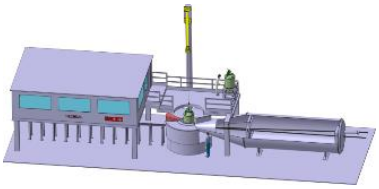
CMC published 127 peer review papers in 2016 covering both new directions and long sought results in key areas. CMC was involved in 12 PhD degrees and 17 Master degrees bringing the cumulative number for 2010-2016 to 753 publications, 3 doctoral, 63 PhD and 94 MSc degrees.

Selected scientific highlights:



Discovery of new light element alkali metal amides

These materials are relevant for direct hydrogen or ammonia storage, ammonia cracking or as ion conductors for batteries. *In-situ* PXRD shows that $Li_3Na(NH_2)_4$ releases $NaNH_2$ and forms non-stoichiometric $Li_{3+x}Na_{1-x}(NH_2)_4$ before it melts at 234 °C (Jepsen *et al.*, *Phys. Chem. Chem. Phys*. **2016**, 18, 1735-1742).

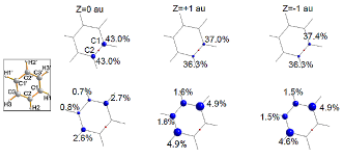


HEIMDAL through ESS scope setting with a budget of 13.55 M€

Heimdal: The thermal neutron powder diffractometer with high and flexible resolution combined with a SANS and neutron imaging set-up designed for the study of materials science at the European Spallation Source (Holm *et al., Nuclear Inst. and Methods in Physics Research A* **2016**, 828, 229-241).

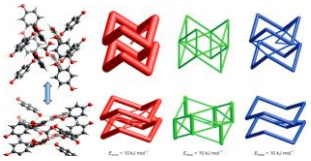
Source Function reveals subtle electron delocalization effects

Experimental Source Function patterns in molecular crystals detect subtle electron delocalization effects and assess their transferability properties. The agreement with corresponding patterns from crystal periodic ab-initio wavefunctions is impressive (Gatti *et al.*, *Acta Crystallographica B* **2016,** 72, 180-193 (invited Feature article)).



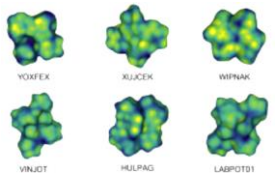
ECC DOSY NMR enables studies of aggregation/deaggregation in solution

Studies have uncovered e.g. whether catalysis is conducted by a mononuclear or by a polynuclear organometallic species, if weak interactions are robust enough to be maintained in a particular solvent for a given reaction (Neufeld *et al.*, *J. Am. Chem. Soc.* ***2016****, 138, 4796-4806*; *Chem. Eur. J.* **2016**, *22*, 12624-12628).



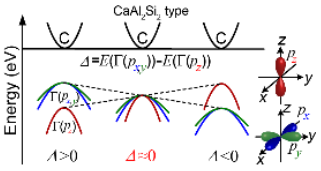
Energy frameworks used to rationalise host-guest interactions

Intermolecular interaction energies in the hydroquinone – formic acid clathrate help explain trends in guest inclusion and the origin of a pressure medium dependent phase transition (Eikeland *et al.*, *Chem. Eur. J.* **2016**, 22, 4061-4069).



Profiling of molecular shapes in crystals

The rotation invariant description of molecular shapes e.g. Hirshfeld surfaces via spherical harmonic functions constitutes an efficient and effective technique for incorporating molecular shape into the statistical/quantitative analysis of experimental crystal structures. (Spackman *et al.*, Sci. Rep. **2016**, 6:22204).

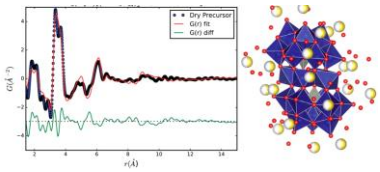


Designing high-performance thermoelectric materials by orbital engineering

Theoretical prediction of new layered thermoelectric materials is now possible through a new measure based on orbital degeneracy providing a clear link between properties and crystal structure (Zhang *et al.*, *Nature Commun.* **2016**, 7, 10892).

Chemistry of nucleation

Atomic scale insight into the nucleation of crystals may provide a paradigm shift in nucleation theory. Elaborate in situ PDF analysis revealed that a large Tourne-type sandwich complex is the precursor for $ZnWO_4$ nanocrystal formation (Bøjesen *et al., Chem. Sci.* **2016**, **7**, 6394 - 6406).



Crystal structure of thermoelectric SnTe

Tin and lead chalcogenides exhibit the highest known thermoelectric figures of merit. Anharmonicity in SnTe was studied by NXMEM analysis and a long debated low temperature phase transition was rejected based on synchrotron X-ray diffraction analysis (Sist et al., *IUCr-J* **2016**, 3, 377-388).