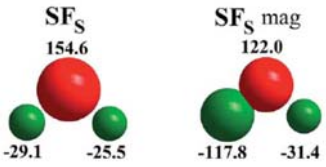
Center for Materials Crystallography: Highlights in 2015

CMC published 99 peer review papers in 2015 and as in previous years many studies were reported in international top journals. The long term impact was further strengthened with awarding 1 doctoral degree, 9 PhD degrees and 22 Master degrees. Thus, the cumulative number for 2010-2015 is 626 publications, 3 doctoral, 52 PhD and 87 MSc degrees.

Selected scientific highlights:

Insights on spin polarization through the spin density source function

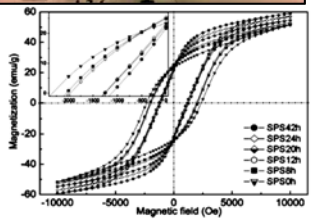


Understanding transmission of spin information from paramagnetic to non-magnetic centers is crucial in advanced materials research. A novel tool has been developed to e.g. quantify atom contributions to spin polarization (Gatti *et al*., *Chem. Sci.* **2015**, 6, 3845-3852).

In situ X-ray diffraction environments for high-pressure reactions

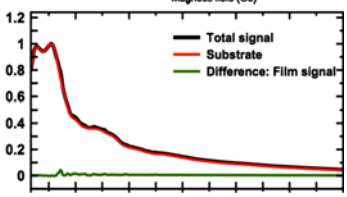
New sample environments and techniques customized for *in situ* powder X-ray diffraction studies up to 1000 bar gas pressure were developed. The cells can be utilized for multiple purposes in a range of research fields (Hansen *et al., J. Appl. Cryst*. **2015**, 48, 1234–1241).

High Alignment of magnetic $SrFe_{12}O_{19}$ nanoplatelets by Spark Plasma Sintering



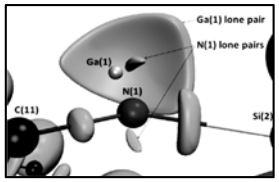
Spark plasma sintering has been used to compact $SrFe_{12}O_{19}$ powders into a quasi-single crystal with an almost completely aligned c-axis observed by measurement of magnetic properties and pole figures from XRD (Stingaciu *et al., Sci. Rep.* 2015, **5**, 14112; Saura-Múzquiz et al., *Nanoscale* **2016**, DOI: 10.1039/C5NR07854G).

Thin film pair distribution function analysis demonstrated for the first time



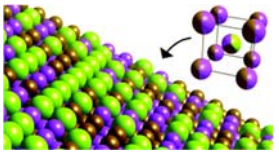
Local atomic structure has for the first time been determined in amorphous and crystalline thin films by PDF analysis. The breakthrough was the use of transmission geometry, which allows analysis of even extremely weak sample signals (Jensen *et al*., *IUCR-J* **2015**, 2, 481-489; Bauers *et al*., *J. Am. Chem. Soc.* **2015**, 137, 9652–9658).

Chemical Bonding and Electronic Localization in a Ga^{I} Amide



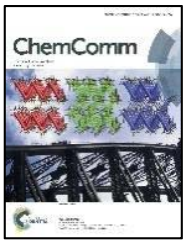
The electron density in a [GaIN(SiMe3)R] complex has been determined from *ab initio* calculations and multipole modeling of 90 K XRD data. Electron density analysis suggests a reversal of bonding roles with an electron donating metal (Thomsen *et al*., *Chem. Eur. J.* **2015**, 21, 14460-14470).

High-pressure phase transitions in ordered and disordered Bi_2Te_2Se



High pressure XRD studies of the topological insulator and thermoelectric Bi_2Te_2Se revealed an electronic transition followed by two structural transitions leading to an unusual disordered alloy (Nielsen *et al.*, Dalton Trans. **2015**, 44, 14077-14084).

Novel method to estimate nuclear densities from X-ray data - NXMEM

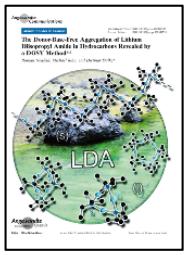


A method to derive nuclear weighted MEM electron densities was developed and tested on high performance thermoelectric materials containing subtle disorder. The general method provides a highly significant improvement to normal maximum entropy method analysis (Christensen *et al.*, *Acta Crystallogr. Sect. A* **2015**, 71, 9–19).

Rationalising mechanical behaviour of molecular crystals at a molecular level

Combining model interaction energies with a novel graphical representation of their magnitude – *energy frameworks* – addresses intriguing questions about the mechanical behavior of crystals (Turner *et al., Chem. Commun.* **2015**, 51, 3735).

DOSY-NMR used to probe organometallic aggregation behaviour



Lithium diisopropyl amide is one of the most common non-nucleophilic Brønsted bases in industry, but its aggregation in donor-base free solvents has so far been unclear. A new DOSY-NMR method quantifies the aggregation in solution (Neufeld et al., *Angew. Chem. Int. Ed.* **2015**, *54*, 6994-6998).