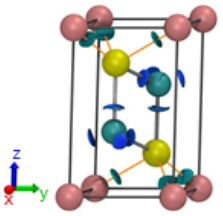
Center for Materials Crystallography: Highlights in 2018

In 2018, CMC published 104 peer reviewed papers in high impact journals covering both broad interest and niche subject matter. CMC was involved in the awarding of 8 PhD degrees and 20 Master degrees. Selected scientific highlights are given below:

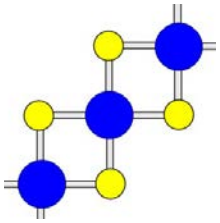
Alleviating frustration over frustrated magnets

The 3D-mΔPDF technique was employed to directly determine magnetic correlations in Bixbyite from experimental data. For the first time, we demonstrated the quantification of magnetic correlations in frustrated magnets from neutron diffraction data, making no prior assumptions about the structure. (Roth et al., *IUCr-J*, 5, **2018**, 410)



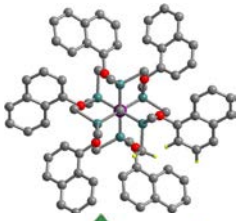
Thermoelectrics of the Future

Lack of anisotropy in the thermoelectric properties of Mg_3Sb_2 were determined to arise from the crystal structure; a study that also challenged the very nature of the commonly accepted Zintl model. Instead, the interlayer interaction was determined to be ionic with partial covalent nature. (Zhang et al., Nature Comm., **9**, 2018, 4716)



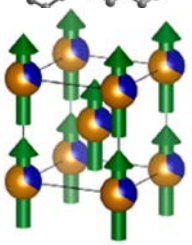
A benchmark method for Van der Waals solids

Weak interlayer interactions in TiS_2 were discovered to possess more electron deformation from synchrotron X-ray diffraction data with respect to theoretical findings. This is an important development for understanding this class of materials, where knowledge of weak bonding interactions from experimental data offer insight in to performance of real materials. (Kasai et al., *Nature Materials* **2018**, 17, 249)



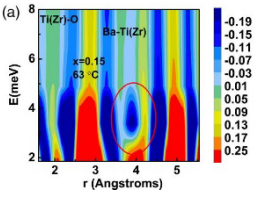
Molecular magnets by design

An extreme coordination environment was found to confer f-element-like electronic structure on a linear cobalt(II) complex, revealing a method by which the magnetic coercivity may be enhanced in transition metal complexes. (Bunting et al. *Science*, **2018**, 362, 1378)



Nano-magnets

A multi-technique composition analysis of magnetic nanocomposites determined that the reduction of the single-phase $CoFe_2O_4$ spinel to pure metallic alloy proceeds via a Co-rich phase, leaving a residual Co-deficient spinel. Preparation at a lower temperature was determined from this study to minimize the Co deficient phase formation and thus inhibit magnetic softening. (Granados Miralles et al., *ACS Appl. Nano Mater.* **2018**, 1, 3693)

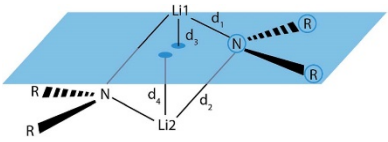


Disorder in Functional Ferroelectrics

Pb-free ferroelectrics were examined by the dynamic pair distribution function to understand the nature of local dipole-dipole correlations in polar nanoregions; an important structural phenomenon which impacts their functionality. (Pramanick et al. *Physical Review Letters*, **2018**, 120, 207603)

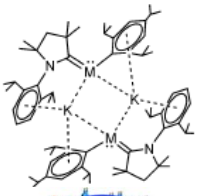
Amide vs. Amine

The ionic (71-72 %) and covalent (25-26 %) character of the Li-N bond were found to be in stark contrast to the old dichotomy of 95-5% through a thorough experimental an theoretical study on $[\{(Me_2NCH_2)_2(C_4H_2N)\}Li]_2$. (Engelhardt, et al. *Chem. Sci.* **2018**, 9, 3111-3121)



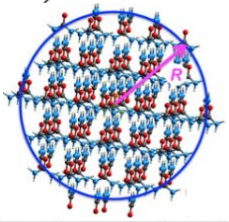
Isolating Anions

Isolation of the cAAC-stabilized silanylidene (II) and germanylidene (III) anions was performed for the first time, and consolidated by both experimental analysis and theoretical examination of the structure and bonding. (Siddiqui et al., *Angew. Chem. Int. Ed.* **2018**, 57, 11776-11780)



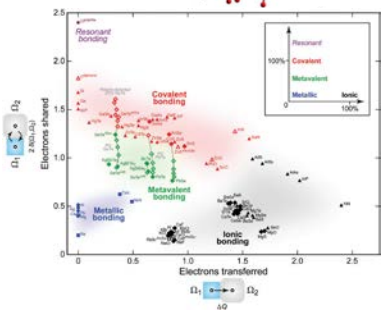
Confidence in Lattice Energy Prediction

A combination of CE-B3LYP model energies and experimental crystal structures were used to establish a level of confidence for lattice energies. Based on this work, it was noted that the interpretation of calculations via different methods from different crystal/molecule geometries should be treated with care. A lack of benchmark data sets was also highlighted, particularly for organic molecules. (Thomas et al., J. *Chem. Theory Comput.* **2018**, 14, 1614-1623)



Mapping Materials

2D maps of solid state materials have been generated from a quantum-mechanical description of electron sharing and transfer, where a third dimension (namely physical properties) may be applied to allow tailoring of material properties. (Raty et al. *Adv. Mater.* **2018**, 1806280)



Influence of face to face monomer π–π overlap on heterocyclic systems

Optically biaxial single crystals of the heterocyclic system 5,6,10b-triazaacephenanthrylene (TAAP) were shown to exhibit absorption and fluorescence anisotropy upon JH-aggregation with a face-to-face alignment of monomers in centrosymmetric dimers. This interaction was found to determine the crystal packing and orientation of the absorption and emission transition dipole moments. (Ostrowska et al., *IUCrJ* **2018** 5, 335-347)