

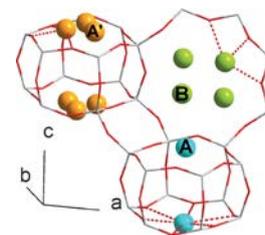


Center for Materials Crystallography: Highlights in 2017

CMC published 111 peer review papers in 2017 covering both new directions and long-sought results in several key areas. CMC was involved in the awarding of 19 PhD degrees and 11 Master degrees. Selected scientific highlights are given below:

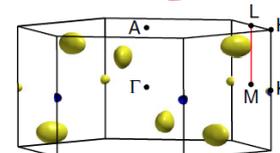
New insight in zeolite catalysis

Quasi-simultaneous PXRD and XANES yielded the first insight into the correlation between oxidation state and migration of Cu⁺-ions in the commercially important zeolite Cu-CHA (Andersen *et al.*, *Angew. Chem. Intl. Ed.*, 56, **2017**, 10367)



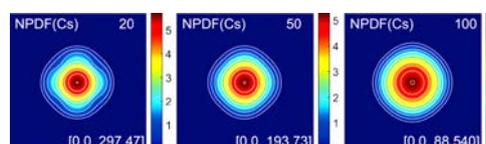
Novel thermoelectric material discovered

Multi-valley band engineering was used to develop Te-doped Mg₃Sb_{1.5}Bi_{0.5}, a groundbreaking new n-type thermoelectric material (Zhang *et al.*, *Nature Comm.*, **2017**, 8, 13901)



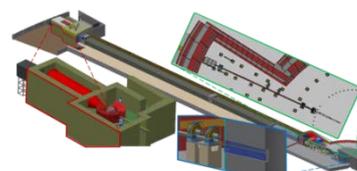
News for the textbooks

The unusually low thermal conductivity in the simple defect free cubic crystal of CsCl is a puzzle. Peculiar anharmonic motion of Cesium is observed at low temperature (Sist *et al.*, *Angew. Chem. Intl. Ed.*, 56, **2017**, 3625)



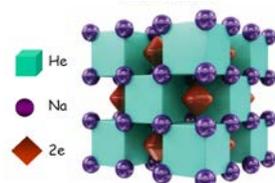
Tollgate 2 passed for HEIMDAL

More than 250 page documentation laid the ground work of HEIMDAL@ESS to pass the tollgate 2. The instrument is now in the “detailed design” phase.



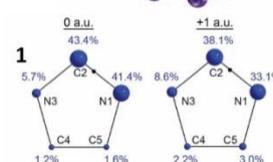
The last bastion of chemical inertness has finally fallen

CMC theoreticians have contributed to the discovery of the first stable compound of Helium and Sodium, Na₂He, which forms at high pressure, >113 GPa. (Dong *et al.*, *Nature Chemistry*, **2017**, 9, 440–445)



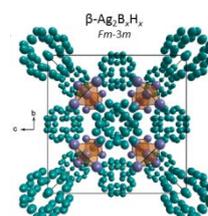
Imidazole and imidazolium scrutinized

Charge density analysis and theoretical calculations have convincingly shown how cyclic π -electron delocalization in the N-heterocyclic rings of related imidazole and imidazolium compounds are much more similar than previously thought (Overgaard *et al.*, *Chem. Eur. J.*, 2018, 24; submitted 2017).



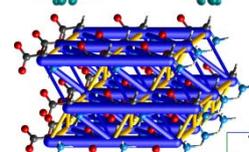
Previously unknown class of silver-based semiconductors discovered

A novel class of semiconducting silver closo-boranes, Ag₂B₁₀H₁₀ and Ag₂B₁₂H₁₂, with a bandgap at 2.3 eV and extremely high ion conductivity were discovered and structurally characterised (Paskevicius *et al.*, *Nature Comm.*, **2017**, 8, 15136, 1-6).



CrystalExplorer model energies and energy frameworks

CrystalExplorer was extended to metal coordination compounds, organic salts, solvates and open shell systems (Mackenzie *et al.*, *IUCr J.*, **2017**, 4, 575-587).



Fire and water unified

CMC succeeded in synthesizing a unique, water-stable yet reactive organopotassium compound, [(18-crown-6)K{(4,6-*t*Bu-OCNC₆H₂)₂CH}•H₂O] (Koehne *et al.*, *Angew. Chem. Intl. Ed.* **2017**, 56, 15141-15145)

