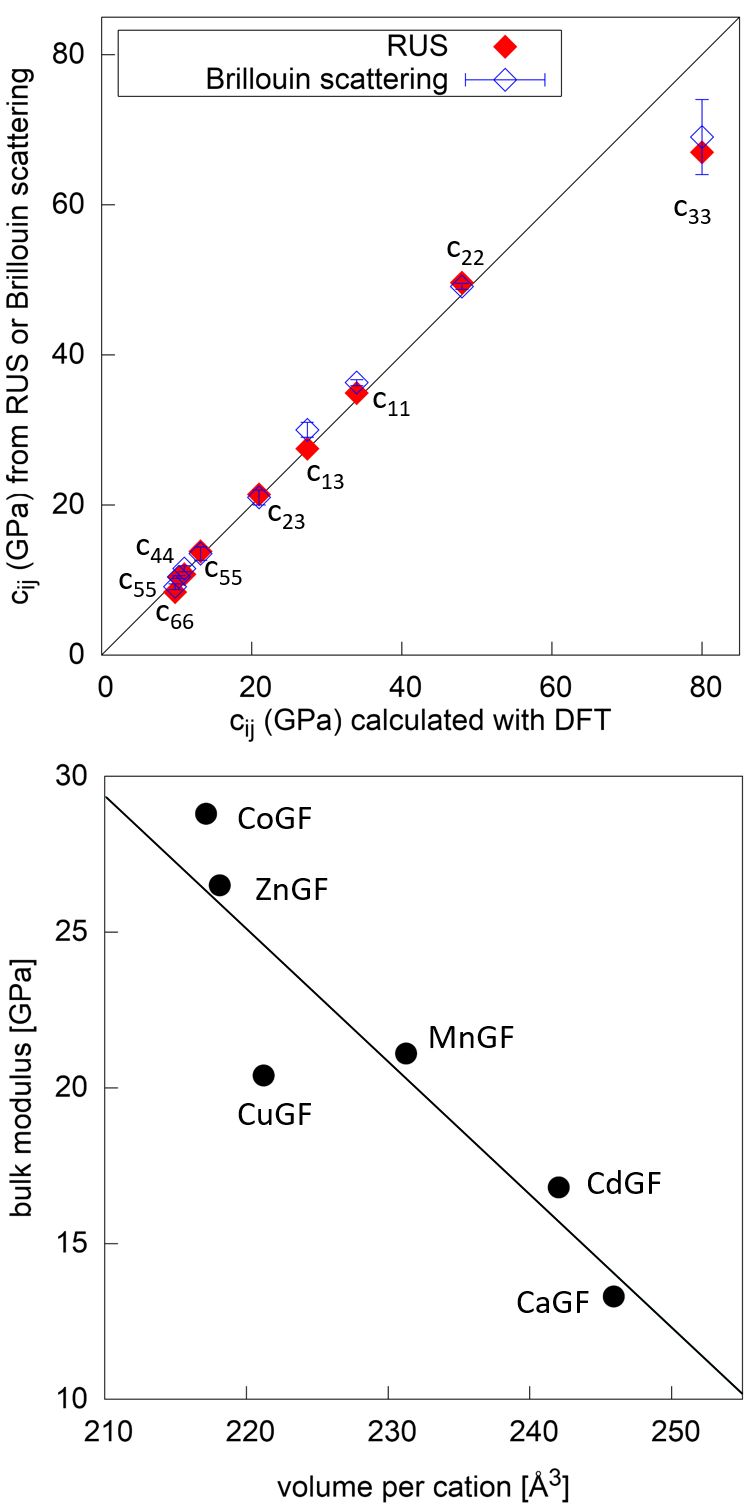
**Elasticity of dense metal-organic framework compounds**

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Metal-organic framework (MOF) compounds are a class of promising crystalline microporous materials containing metal ions coordinated by organic linkers. Among the various MOF structures, perovskite-like structured MOFs have attracted attention due to their chemical diversity and their potential for a number of applications, e.g. in photovoltaic energy generation [1].

In the present study, the elastic behavior of metal-guanidinium formates (*M*GF), where *M*= Cu, Zn, Mn, Co, Ca and Cd has been investigated. This is of interest as these MOFs are known to undergo magnetic and/or structural phase transitions at low temperatures [3,4,5] and their elastic stiffness tensors may provide insight into the origin of their ferroic or multiferroic behavior.

*M*GFs are perovskite-like MOFs. Their general formula is ABX3, where A represents C(NH2)3, B is a divalent metal ion (*M* = Cu, Zn, Mn, Co, Ca or Cd), and X is the polyatomic linker anion, formate = HCOO-. The elastic properties of ZnGF, MnGF, CoGF and CuGF have been investigated by plane wave / parallel plate ultrasound spectroscopy, resonant ultrasound spectroscopy (RUS), Brillouin spectroscopy (BS), density functional theory, and the analysis of thermal diffuse scattering.

Fig.1 Top: cij for ZnGF obtained by DFT compared to those obtained by RUS and BS. Experimental values on the black line indicate perfect agreement with the results from DFT. Bottom: Bulk modulus of the MGF as a function of volume of their unit cells per cation.

Fig. 1 shows a comparison of the experimental results to DFT-results for ZnGF. There generally is a good agreement between the different techniques and the theoretical data, if dispersion-corrected DFT calculations are employed. The *M*GFs crystallize in different structure types, where ZnGF, MnGF and CoGF are isostructural. The structure of CuGF only differs slightly from that of ZnGF [3], while CdGF and CaGF have distinct structures [4, 5]. Our results show a systematic variation of the bulk modulus as a function of the radius of the *M*-cation, which leads to the conclusion that at ambient conditions the elastic behavior is mainly due to the packing density and depends little on the bonding between the *M*-cation and the formate.

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EH and JB are grateful for funding from the DFG (HA 5137-5) BW and LP thank the DFG for funding in Wi 1232. KB thanks the GSI (Darmstadt) for financial support. BW is grateful for support through the BIOVIA Science Ambassador program.