MS13 Structural Characterization of Functional Materials

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Structural Chemistry of ABX3 Molecular Perovskites
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Abstract
A recent research direction related to ABX_3 perovskites is the use of molecules on the A and/or X-site, a development that has proved fruitful for photovoltaics, (improper) ferroelectrics and barocalorics. Replacing atoms by molecules increases the chemical space for the synthesis of materials with new properties, conceptually translating chemical, synthetic freedom to novel opportunities in material design. In my presentation I will discuss how the use of molecular building units in molecular materials introduces new structural degrees of freedom of rotational, translational, and conformational nature that can be exploited for material design. I will discuss how understanding and controlling these structural degrees of freedom is key for efficiently harnessing their chemical diversity by drawing on my group's recent research results such as the discovery of a new type of polymorphism in ABX_3 molecular perovskites, the application of information theory to calculate the complexity of (molecular) perovskites, and how to integrate new geometric degrees of freedom through the use of divalent A^{2+} cations.

References
[1] S. Burger, S. Grover, K. T. Butler, H. L. B. Boström, R. Grau-Crespo, G. Kieslich. Tilt and Shift Polymorphism in Molecular Perovskites. *Mater. Horiz*. **2021**, 8, 2444.
[2] S. A. Hallweger, C. Kaußler. The structural complexity of perovskites. *Phys. Chem. Chem. Phys*. **2022**, 24, 9196.
[3] S. Burger, K. Hemmer, D. C. Mayer, D. Daisenberger, J. K. zareba, G. Kieslich. Designing Geometric Degrees of Freedom in ReO3-type coordination polymers. **2022**, *ChemRxiv*: 10.26434/chemrxiv-2022-mkcw8.