The Evolution of Perovskite Complexity

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What is the complexity of a crystal structure? From a structural chemist's perspective, the complexity of a crystal structure is linked to the amount of information that is required to describe a crystal structure, implicitly defining a rating scheme for complexity: the crystal structure's information content. This idea is in the centre of a recent approach as developed by S. V. Krivovichev[1] where the crystallographic information file is seen as a message. By using established formulas from information theory, its information content is extracted, providing a framework to differentiate between the complexity of crystal structures.

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 apply an information theory-based approach[1,2,3] and discuss the evolution of crystal structure complexity across several perovskite classes such as oxide perovskites, hybrid-organic inorganic perovskites, and molecular perovskites. I will show that increased chemical diversity is synonymous with increased structural complexity which scales with the size of the pseudocubic ReO_3-type network and available distortions schemes. The complexity analysis applied here provides a new perspective on the crystal chemistry of perovskites and shows a large potential for rationalizing the role of configurational entropy in understanding temperature-driven phase transitions. I will close the presentation by overviewing recent theory developments that implicate the use of crystal structure complexity in research areas such as barocalorics and crystal growth processes amongst others.

[1] S. V. Krivovichev, *Angew. Chem. Int. Ed*. **2014**, 53, 654.

[2] C. Kaußler, G. Kieslich *J. Appl. Cryst*. **2021**, 54, 306.

[3] http://www.github.com/GKieslich/crystIT/