Octahedral Tilting, Cation Ordering, And Hydrogen Bonding in Layered Hybrid Halide Perovskites

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Layered hybrid halide perovskites consist of layers of corner connected metal halide octahedra separated by organic cations. This class of materials can be further divided into compounds that adopt the Ruddlesden-Popper (RP) structure, where the octahedra in neighboring layers are offset from one another and those that adopt the Dion-Jacobson (DJ) structure, where the octahedra in neighboring layers lie directly over one another. In this talk I will discuss our studies of the structures of hybrid organic-inorganic layered perovskites. Using the tools of group theory, we have mapped out the symmetry consequences of structural distortions in this class of materials. These distortions include octahedral tilting, cation ordering within the inorganic layers, and orientational ordering of the organic cations. The combined analysis shows that certain modes of octahedral tilting are strongly favored in large part because they lead to favorable hydrogen bonding interactions between the halide ions of the inorganic layers and organic cations that sit between the layers. This information is used to guide our search for new lead-free ferroelectrics, piezoelectrics, and multiferroics. A better understanding of the forces that drive phase transitions in this family is also likely to have utility for the design of new barocaloric materials.

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