Hexagonal and Versus SrMnO3: Band Structure, Heat Capacity and Lattice Dynamics

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Hexagonal perovskites in which octahedra share faces (alternating face and corner sharing layers) and form chains along the hexagonal c-axis are less common than cubic perovskites where all octahedra share corners and typically form when the A-site cations (i.e. Sr in our case) are too large for the ideal cubic perovskite structure. Thus the majority of the hexagonal perovskites contain large alkali or alkali-earth metals in the A-site and transition metals in the B-site. The hexagonal perovskites are stabilized by the formation of metal-metal bonds between the B-cations of the BX6 octahedra which are strong enough to overcome metal-metal repulsion between A cations. SrMnO3 is a rare example of a compound taking both structures. A hexagonal modification is stable up to 1300K where it transforms to a cubic high temperature modification. Several factors contribute to the relative stability of the two polymorphs.

In this contribution we focus in part on electronic contributions to the phase stability through first-principles density functional theory (DFT) within the projector augmented wave (PAW) framework and in part on subsequent studies of the lattice dynamics. These calculations are compared with experimental heat capacities using Quantum Designs relaxation calorimeter.