

Effect of cation ordering and pressure on n=2 Ruddlesden-Popper oxides from first principles

Sriram P Ramkumar and Elizabeth A Nowadnick

Department of Physics, New Jersey Institute of Technology, University Heights,
Newark, New Jersey 07102 (USA)

Octahedral tilts and rotations are ubiquitous in perovskite oxides and couple strongly to the electronic and magnetic properties. In n=2 Ruddlesden-Popper (RP) $A_3B_2O_7$ layered perovskites, two octahedral rotations of different symmetries can induce a polarization via a trilinear coupling mechanism, known as hybrid improper ferroelectricity (HIF) [1]. Octahedral rotations can be controlled by various knobs such as chemical substitution, pressure, strain, and explored extensively in ABO_3 perovskites [2]. We perform first-principles density functional theory calculations for a range of RPs. We explore two different approaches for engineering octahedral rotations as well looking at polar (P) to non-polar (NP) phase transition: (1) based on A-site cation ordering (e.g. $A_2A'B_2O_7$), and (2) by the application of hydrostatic pressure.

[1] N. A. Benedek et al., Phys. Rev. Lett. 106, 107204 (2011)

[2] X. J. Xiang et al., Phys. Rev. B 96, 054102 (2017); J. Rondinelli et al., Adv. Mater. 23, 3363 (2011)