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Study of oxygen octahedra rotations in Ruddlesden-Popper phases of perovskite materials JEEHYE LEE, TOMAS ARIAS, Cornell University — We present the most systematic theoretical study of Ruddlesden- Popper(RP) phases in perovskites ($Sr_{n+1}Ti_nO_{3n+1}$ and others) to date. Consistent with experimental results, we find that the formation of stacking faults is energetically favored for certain rotational reconstructions of the bulk material. In particular, we enumerate the set of possible rotational configurations of oxygen octahedra next to the stacking fault and then reduce this set to a subset of distinct configurations by considering the symmetries of the RP structure. For this reduced set, we calculate the formation energy of stacking faults, and study the interaction between separated faults. We find that the planar faults attract each other, and that the interaction energy scales as the inverse distance between the faults.

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