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Alternative techniques to stabilize highly polar $BiFeO_3$-type phase in Pnma perovskites

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BO_6 octahedron rotations are common but very important structure distortions in the ABO_3 perovskite family of compounds[1, 2], that can strongly couple with lattice, electronic structure, magnetism and ferroelectricity. Most of the perovskite compounds adopt the Glazer $a^-a^-c^+$ rotation pattern, where this pattern strongly suppresses the ferroelectric modes[3, 4], leading a structure to stabilize in non-polar Pnma phase. However, there is a small fraction of perovskite compounds with R3c phase that has a $a^-a^-a^-$ rotation pattern which can be favorable to induce large polarization, such as $LiNbO_3$ and $BiFeO_3$[5–7]. Experiments have already discovered and synthesized many ferroelectric and multiferroic materials with R3c phase under high-pressure conditions[8], but such R3c phase materials stabilized under high pressure can not be widely used for practical application. In our study, we find a series of Pnma phase perovskite materials, which exhibit a metastable R3c phase. They can be stabilized to have a stable R3c-like phase under normal pressure condition[9], induced under strain, electric field and interface effect. We also explain the physical mechanism for this phase transition and propose a general rule to discover materials for which R3c-like phase can be induced. we hope these alternative techniques will be useful to find more $BiFeO_3$-like multiferroic materials for materials applications in the future.

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