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A new class of in-plane Ferroelectric Mott insulators via oxide heterostructuring[1] CHANUL KIM, Columbia Univ, HYOWON PARK, University of Illinois at Chicago, CHRIS MARIANETTI, Columbia Univ, MARIANETTI GROUP TEAM[2] — We propose simple design rules based on charge transfer, cation ordering, and size mismatch to design a new class of in-plane ferroelectric Mott insulators in perovskite-based transition metal oxides. Ab Initio DFT+U calculations are then used to selectively scan phase space based on these rules. We begin by exploring pairs of A-type ions (A, A') and pairs of B-type ions (B, B') in $AA'BB'O_6$ which will have nominal charge transfer consistent with valencies that are conducive to a low Mott gap insulator. Additionally, the A-type ions are chosen to have a large size mismatch and stereochemical effect. The ordering of A/A' and B/B' still retains C_{4v} symmetry which may be spontaneously broken to yield an in-plane ferroelectric. We uncover a number of materials which are strong candidates to be in-plane ferroelectric Mott insulators in experiment, including $BaBiVCuO_6$, $BaBiVNiO_6$, $PbLaVCuO_6$. Finally, we will discuss potential applications of in-plane ferroelectric Mott insulators such as ferroelectric photovoltaics, Mott FET, and optoelectronic devices.

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