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A new class of polar mott-insulators via heterostructruring[1]
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— We propose simple design rules based on charge transfer and ion size to design a new class of polar Mott insulators in perovskite-based transition metal oxides. Ab Initio DFT+U calculations are then used to selectively scan phase space in double perovskites which have strong potential to be polar and Mott insulating. 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 Mott insulator. Additionally, the A-type ions are chosen to have a large size mismatch and are ordered to break symmetry, creating conditions favorable to a polar distortion. We uncover a number of materials which are strong candidates to be polar Mott insulators in experiment, including $BaLaVNiO_6$, $BaLaVCoO_6$, $BaLaVCuO_6$, $BaLaCrNiO_6$, $BaBiVCoO_6$, $BaBiVNiO_6$, and $PbLaVNiO_6$. Furthermore, we show that the magnetic state and the band gap are sensitive to the particular ordering of the transition metals. Finally, we discuss possible applications and the potential to grow these systems in experiment.

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