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Design of new Mott multiferroics via complete charge transfer: promising candidates for bulk photovoltaics[1] HANGHUI CHEN, NYU-ECNU Institute of Physics, ANDREW MILLIS, Columbia University — Optimal materials to induce bulk photovoltaic effects should lack inversion symmetry and have an optical gap matching the energies of visible radiation. Ferroelectric perovskite oxides such as $BaTiO_3$ and $BiFeO_3$ exhibit substantial polarization and stability, but have the disadvantage of excessively large band gaps. We use both density functional theory and dynamical mean field theory calculations to design a new class of Mott multiferroics–double perovskite oxides A_2VFeO_6 (A=Ba, Pb, etc). While neither perovskite AVO_3 nor $AFeO_3$ is ferroelectric, in the double perovskite A_2VFeO_6 a 'complete' charge transfer from V to Fe leads to a non-bulk-like charge configuration–an empty V-d shell and a half-filled Fe-d shell, giving rise to a polarization comparable to that of important ferroelectrics $ATiO_3$. Different from nonmagnetic $ATiO_3$, the new double perovskite oxides have an antiferromagnetic ground state and around room temperatures, are paramagnetic Mott insulators. Most importantly, the V d^0 state significantly reduces the band gap of A_2VFeO_6, making it smaller than that of $ATiO_3$ and $BiFeO_3$, which renders the new multiferroics a promising candidate to induce bulk photovoltaic effects.

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