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**New highly polar semiconductor ferroelectrics for solar energy conversion devices** ANDREW M. RAPPE, ILYA GRINBERG, JOSEPH W. BENNETT, University of Pennsylvania — Solar energy is a promising long-term solution for future energy requirements; however, current solar energy conversion devices are plagued by low efficiency. The use of ferroelectric  $ABO_3$  perovskite oxides is one approach for boosting conversion efficiency. Ferroelectric oxides possess spontaneous polarization and have been shown to produce a bulk photovoltaic effect, in which charged carriers, specifically electrons and holes, separate to prevent recombination. Once separated, the high-energy electrons are available for electrical work or for the catalytic splitting of water into hydrogen and oxygen. Currently, most solid oxide ferroelectrics have a band gap of at least 3 eV, absorbing primarily in the ultra-violet (UV) region. Since UV light comprises only 8% of the solar spectrum, new materials with a decreased band gap and large polarization would be highly desirable. We use first-principles density functional theory (DFT) calculations to investigate the ground state structures of  $PbTiO_3$  solid solutions containing Ni, Pd and Pt. We predict that these proposed materials will display a decreased band gap when compared to  $PbTiO_3$ , while maintaining or enhancing polarization. They are promising candidates for use as semi-conducting ferroelectric substrates for solar conversion devices.

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