

Abstract Submitted  
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**Semiconducting ferroelectrics for photovoltaics through Zn<sup>2+</sup> doping into KNbO<sub>3</sub>** FENGGONG WANG, ILYA GRINBERG, PETER DAVIES, ANDREW RAPPE, Univ of Pennsylvania, RAPPE GROUP TEAM, DAVIES GROUP TEAM — Using first-principles calculations, we design and predict six low band gap ferroelectric solid solutions by partially substituting Zn<sup>2+</sup> for Nb<sup>5+</sup> into the parent KNbO<sub>3</sub> material, combined with charge compensations at the *A*-sites by different combinations of higher valence cations (Ba<sup>2+</sup>, Sr<sup>2+</sup>, Pb<sup>2+</sup> and La<sup>3+</sup>, Bi<sup>3+</sup>). In particular, our HSE06 calculations yield a low band gap of only 2.11 eV for the 75%KNbO<sub>3</sub> – 25%(Sr<sub>1/2</sub>La<sub>1/2</sub>)(Zn<sub>1/2</sub>Nb<sub>1/2</sub>)O<sub>3</sub> (KN-SLZN) solid solution, and this can be lowered further by 0.6-0.7 eV upon in-plane compressive strains, allowing for more efficient visible light photovoltaic energy harvesting. The maintaining or enhancing of the polarizations of KN-SLZN provides an efficient charge separation route by the bulk photovoltaic effect that could make the power conversion efficiency (PCE) go beyond the Shockley–Queisser limit. We argue that these newly designed low band gap ferroelectric solid solutions can be experimentally synthesized and are promising for photovoltaics. In addition, we demonstrate a new strategy to engineer the band gap while maintaining the polarization of the ferroelectric perovskites, which can be well applied to other systems.

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