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Photovoltaic properties of low band gap ferroelectric perovskite oxides XIN HUANG, Southeast University, TULA PAUDEL, University of Nebraska-Lincoln, SHUAI DONG, Southeast University, EVGENY TSYMBAL, University of Nebraska-Lincoln — Low band gap ferroelectric perovskite oxides are promising for photovoltaic applications due to their high absorption in the visible optical spectrum and a possibility of having large open circuit voltage. Additionally, an intrinsic electric field present in these materials provides a bias for electron-hole separation without requiring p-n junctions as in conventional solar cells. High quality thin films of these compounds can be grown with atomic layer precision allowing control over surface and defect properties. Initial screening based on the electronic band gap and the energy dependent absorption coefficient calculated within density functional theory shows that hexagonal rare-earth manganites and ferrites are promising as photovoltaic absorbers. As a model, we consider hexagonal $TbMnO_3$. This compound has almost ideal band gap of about 1.4 eV, very high ferroelectric Curie temperature, and can be grown epitaxially. Additionally hexagonal $TbMnO_3$ offers possibility of coherent structure with transparent conductor ZnO. We find that the absorption is sufficiently high and dominated by interband transitions between the Mn d-bands. We will present the theoretically calculated photovoltaic efficiency of hexagonal $TbMnO_3$ and explore other ferroelectric perovskite oxides.

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