

Abstract Submitted
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First-principles materials design of high-performing bulk photovoltaics with the LiNbO₃ structure STEVE YOUNG¹, FAN ZHENG, ANDREW RAPPE, University of Pennsylvania — The bulk photovoltaic effect describes the ability of inversion symmetry breaking materials to produce intrinsic photocurrents and photovoltages. Recently, we have previously demonstrated the ability to compute, from first principles, the bulk photocurrent using the theory of “shift current,” and have successfully reproduced experimental results. This ability has allowed for understanding of the structural and chemical properties generating large bulk photovoltaic response and the design of high-performing materials. In this talk we present three polar oxides with the LiNbO₃ structure that we predict to have band gaps in the 1-2 eV range and very high bulk photovoltaic response: PbNiO₃, Mg_{1/2}Zn_{1/2}PbO₃, and LiBiO₃. The first is has already been synthesized, and the others are very similar to known materials. All three have band gaps determined by cations with $d^{10}s^0$ electronic configurations, leading to conduction bands composed of cation s -orbitals and O p -orbitals. This both dramatically lowers the band gap and increases the bulk photovoltaic response by as much as an order of magnitude over previous materials, demonstrating the potential for high-performing bulk photovoltaics.

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