

Abstract Submitted
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Enhancement of bulk photovoltaic effect in band inversion topological phase transitions LIANG TAN, ANDREW RAPPE, Univ of Pennsylvania — The bulk photovoltaic effect (BPVE) is the generation of photocurrents in the bulk of a single-phase material. The dominant mechanism for the BPVE is the shift current, a non-linear optical effect which involves the excitation of carriers into current-carrying coherent superpositions. This mechanism has a number of advantages over traditional photovoltaics, such as above-band gap photovoltages, and current generation in the bulk. In this work, we show that the shift current BPVE can be enhanced in materials with band inversion topological phase transitions. Using first-principles calculations, we show that the magnitude of the shift current is sharply increased in the vicinity of the band inversion transition, and that the direction of the shift current changes abruptly at the band inversion transition. Taking as examples layered BiTeI and perovskite CsPbI₃, we demonstrate that this effect is robust across different materials systems. To understand these results, we analyze our results using a low-energy effective Hamiltonian and derive the functional form of the shift current lineshape near the band gap energy.

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