

Bulk photovoltaic effect: Nonlinear Optical Contributions

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The physical mechanism for the bulk photovoltaic effect that appears in noncentrosymmetric materials is not well understood. One of the strongest candidates for a truly bulk photovoltaic effect is non linear optical processes - most notably "shift current," which describes the net motion of coherently excited electrons in the absence of inversion symmetry, and has been described analytically several times in the literature. Shift current is also of interest due to the appearance of a phase quantity strongly reminiscent of Berry phase theory. We have developed an expression for shift current suitable for efficient computation utilizing Kohn-Sham eigenfunctions. Our goal is to understand the effect of material and electronic structure on the shift current, as well as determine the extent to which shift current contributes to the bulk photovoltaic effect, and can be used to efficiently harvest energy from visible light.