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Photvoltaic effects in ferroelectrics due to nonlinear optical processes STEVE YOUNG, ANDREW RAPPE, Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania — The physical mechanism for the bulk photovoltaic effect that appears in noncentrosymmetric materials, especially in ferroelectric devices, is not well understood. A promising candidate 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 gauge invariant phase describing the carrier mobility. We have developed an expression for shift current suitable for efficient computation and analysis utilizing wavefunctions of arbitrary origin, and calculated the response for several prominent ferroelectrics – including $LiNbO_3$, $BaTiO_3$, and $PbTiO_3$ – using KS eigenstates. The calculated short-circuit currents appear to be in rough agreement with available experimental results where they exist. Furthermore, they indicate a more subtle relationship between polarization and band gap than has heretofore been presumed, with strong implications for the materials design process, as well as shift current's overall viability as a mechanism for efficiently harvesting solar energy.

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