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The quantitative relationship between polarization differences and the zone-averaged shift photocurrent BENJAMIN FREGOSO, TAKAHIRO MORIMOTO, Univ of California - Berkeley, JOEL E. MOORE, Univ of California - Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory, — A relationship is derived between differences in electric polarization between bands and the "shift vector" that controls part of a material's bulk photocurrent, then demonstrated in several models. Electric polarization has a quantized gauge ambiguity and is normally observed at surfaces via the surface charge density, while shift current is a bulk property and gauge-invariant at each point in momentum space. They are connected because the same optical transitions that are described in shift currents pick out a relative gauge between valence and conduction bands. We treat subtleties arising when there are degenerate bands or points at the Brillouin zone where optical transitions are absent. This relationship means that materials with significant interband polarization differences must have high bulk photocurrent, meaning that the modern theory of polarization can be used as an efficiently calculable means to search for bulk photovoltaic material candidates.

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