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Design principles of shift current photovoltaics[1] ASHLEY COOK, Department of Physics, University of Toronto, Department of Physics, University of California, Berkeley, BENJAMIN FREGOSO, FERNANDO DE JUAN, Department of Physics, University of California, Berkeley, JOEL MOORE, Department of Physics, University of California, Berkeley, Materials Sciences Division, Lawrence Berkeley National Laboratory — While the basic principles and limitations of conventional solar cells are well understood, relatively little attention has gone toward evaluating and maximizing the potential efficiency of photovoltaic devices based on shift currents. In this work, a sum rule approach is introduced and used to outline design principles for optimizing shift currents for photon energies near the band gap, which depend on wavefunctions via Berry connections as well as standard band structure. Using these we identify two new classes of shift current photovoltaics, ferroelectric polymer films and orthorhombic monochalcogenides, both of which exhibit peak photoresponsivities larger than predictions for previously-known photovoltaics of this type. Using physically-motivated tight-binding models, the full frequency dependent response of these materials is obtained. Exploring the phase space of these models, we find photoresponsivities that can exceed 100 mA/W. These results show that considering the microscopic origin of shift current via effective models allows one to improve the possible efficiency of devices using this mechanism and better grasp their potential to compete with conventional solar cells.

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