

Abstract Submitted
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Giant bulk photovoltaic effect and spontaneous polarization of single-layer monochalcogenides¹ TONATIUH RANGEL, Lawrence Berkeley Natl Lab, UC Berkeley, BENJAMIN M. FREGOSO, UC Berkeley, BERNARDO S. MENDOZA, CIO, Mexico, TAKAHIRO MORIMOTO, JOEL E. MOORE, UC Berkeley, JEFFREY B. NEATON, Lawrence Berkeley Natl Lab, UC Berkeley — We implement and use a first-principles density functional theory approach to calculate the shift current response of monolayer group-IV monochalcogenides. We find a larger effective three-dimensional effective polarization (~ 1.9 C/m²) and shift current (~ 200 μ A/V²) than have been previously observed in common ferroelectrics. By using a one-dimensional Rice-Mele tight-binding model we investigate the shift-current tensor along the polarization axis, its relation with polarization, and the conditions under which shift-current reaches a maximum [1]. Importantly, our calculations predict that shift current can be largest in the UV visible range, indicating the potential of these materials for optoelectronic applications.[1] arXiv:1610.06589

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