Abstract Submitted
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Efficient k.p method for first-principles calculation of Seebeck coefficient in quantum transport[1] DAVID A. STRUBBE, Department of Physics, University of California, Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory, SU YING QUEK, Molecular Foundry, LBNL, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University, J.B. NEATON, Molecular Foundry, LBNL, STEVEN G. LOUIE, Dept. of Physics, University of California, Berkeley; Molecular Foundry and Materials Sciences Division, LBNL — Thermoelectric properties of molecular junctions reveal fundamental aspects of nanoscale charge transport at interfaces and are relevant to potential organic/inorganic hybrid thermoelectric materials. Quantum transport calculations typically evaluate the Seebeck coefficient S by finite differences of the transmission as a function of energy. However, in ab initio calculations this quantity is difficult to converge for realistic systems and can require very large k-grids. We derive a new analytic-derivative method to evaluate S via k.p perturbation theory, implement it in a DFT-based scattering-state transport code, and apply it to calculations of molecular junctions. This technique improves k-point convergence by avoiding critical points in the lead bandstructure and allows more efficient calculations of Seebeck coefficients.

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