First-Principles Calculation of Charge Carrier Mobility using Complex Band Structure

Andrew Brooks, Yue Yu, Yuning Wu, Dmitry Skachkov, Hai-Ping Cheng, and Xiaoguang Zhang

Department of Physics, Center for Molecular Magnetic and Quantum Materials and the Quantum Theory Project, University of Florida, Gainesville, FL, 32611-8435

We compute charge carrier mobilities from the complex band structure, using the Quantum Espresso suite. Carriers with finite lifetimes due to scattering may be represented by Bloch states with complex energies. Our method determines the constant complex potential that must be added to a perfect crystal to induce the scattering effects seen in a crystal with defects, which we deduce from a series of complex band calculations. The mean scattering lifetime is computed from the imaginary part of this complex potential, and the carrier mobility is obtained from the scattering lifetime using the Boltzmann transport theory. Mobility is calculated for graphene, hybrid organic-inorganic perovskites as a function of temperature due to phonon scattering, impurity and absorbed molecules.

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