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First-principles calculation of mobility in silicon[1] YUNING WU, Vanderbilt University, X.-G. ZHANG, Oak Ridge National Laboratory, SOKRATES T. PANTELIDES, Vanderbilt University — We introduce a new first-principles method to calculate Coulomb-scattering-limited electron mobility in silicon. The lifetime of a Bloch state due to scattering can be interpreted as arising from an additional imaginary part of electron self-energy. By introducing an artificial imaginary potential, the electron self-energy can be extracted from the complex band structure of a periodic system while eliminating the interference effect due to multiple scattering between impurities. This allows an implementation using density functional theory within the Quantum-Espresso package. The calculated electron mobility agrees with the experimental data.

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Yuning Wu
Vanderbilt University

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