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Ab Initio Simulation of Metal Contacts to 2D Semiconductors with Electron-Phonon Interactions WUSHI DONG, PETER LITTLEWOOD, The University of Chicago — Contact resistance could potentially limit the performance of aggressively scaled devices based on two-dimensional (2D) materials. In this work, we present full-band atomistic quantum transport simulations of metal contact to 2D semiconductors including electron-phonon scattering. A combined approach based on the Keldysh Non-equilibrium Green's Function (NEGF) formalism and a mean-field description of the electronic structure is used to calculate vertical transport in an extended device. Tight-binding parameters and electron-phonon coupling constants obtained through the maximally localized Wannier function technique enable us to model the transport at low computational costs. The long-range polar optical contribution is split from the short-range one in order to properly treat the divergence of the electron-phonon matrix elements at long-wavelength limit. Electron transport is found to happen mainly near the energy range where the bands of metal contact and 2D semiconductor cross. The dependence of contact resistance on the overlap length is also studied to determine the ultimate scalability. Our analysis of transport efficiencies provides the foundation and motivation for experimental works.

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