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Effects of Electron-Phonon Interaction in Graphene: The First Principle Calculation J.T. MULLEN, K.M. BORYSENKO, E.A. BARRY, Y.G. SEMENOV, M. BUONGIORNO NARDELLI, J.M. ZAVADA, K.W. KIM, North Carolina State University — We investigate the electron-phonon interaction in intrinsic monolayer graphene using density functional perturbation theory. These results clearly show that the coupling energy is of the same order for all four in-plane phonon branches. Electron scattering rates calculated based on these matrix elements show the substantial contribution of scattering with optical phonons, as well as intervalley scattering with acoustic phonons at \( T > 200 \) K. Based on obtained “effective” deformation potential constants we suggest that the influence of a substrate in graphene is presently underestimated, which could explain the discrepancies in estimates of deformation potential constant based on available experimental data. The low-field mobilities calculated with the full-band Monte Carlo simulation based on the obtained scattering rates are in agreement with recent experiments.

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