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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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