

Optical Phonon Anomaly in Bilayer Graphene with Ultrahigh Carrier Densities

J.-A. Yan,¹ K. Varga,² and M.-Y. Chou^{3,4}

¹*Department of Physics, Astronomy, and Geosciences,
Towson University, Towson, MD 21252, USA.*

²*Department of Physics and Astronomy, Vanderbilt University, Nashville, TN 37035, USA.*

³*School of Physics, Georgia Institute of Technology, Atlanta, GA 30332, USA.*

⁴*Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan.*

Electron-phonon coupling (EPC) in bilayer graphene (BLG) at different doping levels is studied by first-principles calculations. The phonons considered are long-wavelength high-energy symmetric (S) and antisymmetric (AS) optical modes. Both are shown to have distinct EPC-induced phonon linewidths and frequency shifts as a function of the Fermi level E_F . We find that the AS mode has a strong coupling with the lowest two conduction bands when the Fermi level E_F is nearly 0.5 eV above the neutrality point, giving rise to a giant linewidth (more than 100 cm^{-1}) and a significant frequency softening (60 cm^{-1}). Our ab initio calculations show that the origin of the dramatic change arises from the unusual band structure in BLG. The results highlight the band structure effects on the EPC in BLG in the high carrier density regime.

[1] Jia-An Yan, K. Varga, and M. Y. Chou, <http://arxiv.org/abs/1204.1584>.