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Phonon dispersions and vibrational properties of monolayer, bilayer, and trilayer graphene[1] JIA-AN YAN, W. Y. RUAN, M. Y. CHOU, School of Physics, Georgia Institute of Technology — The phonon dispersions of monolayer and few-layer graphene (AB bilayer, ABA and ABC trilayers) are investigated using the density-functional perturbation theory (DFPT). Compared with the monolayer, the optical phonon E_{2g} mode at Γ splits into two and three doubly degenerate branches for bilayer and trilayer graphene, respectively, due to the weak interlayer coupling. These modes are of various mode symmetry and exhibit different sensitivity to either Raman or infrared (IR) measurements (or both), and therefore the combination of Raman and IR measurements of the zone-center optical modes should give a clear identification of the layer number as well as the stacking geometry. The splitting is found to be 5 cm^{-1} for bilayer and 2 to 5 cm^{-1} for trilayer graphene. The interlayer coupling is estimated to be about 2 cm^{-1}. We found that the highest optical modes at K upshift by about 12 cm^{-1} for bilayer and 18 cm^{-1} for trilayer relative to monolayer graphene. The atomic displacements of these optical eigenmodes are analyzed.

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