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Interaction graphene with metallic and semiconductor surfaces. Ab initio approach to the lattice dynamics[1] ALEJANDRO MOLINA SANCHEZ, LUDGER WIRTZ, University of Luxembourg — The interaction of graphene with substrates can alter its electronic and vibrational properties and is relevant for the practical use of graphene. In this work, we describe the graphene-substrate interaction through the theoretical study of the vibrational properties. We focus on three paradigmatic cases where the interaction strength changes gradually: graphene@BN, graphene@Ir(111), and graphene@SiC. We use *ab initio* methods to obtain the phonon band structure, the density of states, and the strength of the electron-phonon coupling. Graphene on boron nitride exhibits a weak interaction but a non-negligible shift of the 2D Raman band. We explain this observation by connecting the increase of the dielectric screening with the softening of the electron-phonon interaction. Graphene on iridium, also displays weak interaction but the substrate is a metal. In this case the electron-electron interaction in graphene is screened by a metal electron gas. In the last case, we study the buffer layer of graphene on silicon carbide. The strong hybridization of graphene with silicon carbide changes substantially the electronic structure of graphene. All the calculations are compared to experimental data of Raman spectroscopy and angle-resolved inelastic electron scattering.

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