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Vibrational properties in graphene-on-metal systems: A scanning tunneling microscopy study and density functional theory calculations HAIGANG ZHANG, YUYANG ZHANG, WENDE XIAO, SHIXUAN DU, HONGJUN GAO, Institute of Physics, Chinese Acadamy of Science, PROF. HONGJUN GAO'S NANO RESEARCH GROUP TEAM — Combing inelastic electron tunneling microscopy (IETS) measured by scanning tunneling microscopy and quantum mechanical calculations based on density functional theory, we investigate and compare the vibrational properties of graphene on various transition metal substrates. The observed d2I/dV2 spectra and mappings indicate there is a mode dependant spatial localization for graphene on Ru(0001) surface In contrast, vibrations of graphene on Pt(111) surface and Ni(111) surface is homogeneous. Out-of-plane vibration modes of graphene are tuned by the different interactions on these three substrates. Vibrational density of states of graphene and graphene/Ni(111) system are calculated and make comparison to the IETS experiments. We also calculate the inelastic and elastic tunneling coefficients in Graphene/Ni(111) system to understand the missing peak in IETS experiments. Our results point to the importance of interfacial bonding on phonon properties and, consequently, electronic and thermal transport properties of graphene based devices.

Haigang Zhang
Institute of Physics, Chinese Acadamy of Science

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