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First Principles Study of Chemically Functionalized Graphene[1]
SANJIV JHA, IGOR VASILIEV, New Mexico State University — The electronic, structural and vibrational properties of carbon nanomaterials can be affected by chemical functionalization. We applied *ab initio* computational methods based on density functional theory to study the covalent functionalization of graphene with benzyne, carboxyl groups and tetracyanoethylene oxide (TCNEO). Our calculations were carried out using the SIESTA and Quantum-ESPRESSO electronic structure codes combined with the local density and generalized gradient approximations for the exchange correlation functional and norm-conserving Troullier-Martins pseudopotentials. The simulated Raman and infrared spectra of graphene functionalized with carboxyl groups and TCNEO were consistent with the available experimental results. The computed vibrational spectra of graphene functionalized with carboxyl groups showed that the presence of point defects near the functionalization site affects the Raman and infrared spectroscopic signatures of functionalized graphene.

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