

Abstract Submitted
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Ab Initio Study of Graphene Functionalized with Carboxyl Groups and Tetracyanoethylene Oxide¹ SANJIV JHA, IGOR VASILIEV, New Mexico State University, IGOR MAGEDOV², LILIYA FROLOVA, NIKOLAI KALUGIN, New Mexico Tech — The electronic and structural 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 carboxyl (COOH) groups and tetracyanoethylene oxide (TCNEO). Our calculations were carried out using the SIESTA and Quantum Espresso electronic structure codes combined with the generalized gradient approximation and local density approximation for the exchange correlation functional. The calculated binding energies and vibrational spectra of functionalized graphene surface and H-terminated graphene edge were compared with the available experimental data. Our calculation showed that the reaction of cycloaddition of TCNEO to graphene was endothermic for the surface of pristine graphene and exothermic for the edge of H-terminated graphene sheet. The simulated Raman and IR spectra of graphene functionalized with TCNEO were consistent with the experimental results. The computed vibrational spectra of graphene functionalized with COOH groups showed that the presence of point defects near the functionalization site affects the Raman and IR spectroscopic signatures of functionalized graphene.

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