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Functionalization of Boron- and Nitrogen-Doped Graphene and Carbon Nanotubes: An *Ab Initio* Study[1] NABIL AL-AQTASH , IGOR VASILIEV, New Mexico State UniVersity — We study the mechanism of covalent functionalization of boron (B) and nitrogen (N) doped graphene and carbon nanotubes by carboxyl (COOH) groups. Our calculations are carried out using density functional theory combined with the generalized gradient approximation for the exchange-correlation functional. The binding energies and equilibrium geometries of carboxylated B/N-doped graphene sheets and carbon nanotubes are examined in cases of graphene and carbon nanotubes containing no defects, containing Stone-Wales defects, and containing vacancies. Our calculations show that B-doping increases and N-doping decreases the binding energy of COOH groups to defect-free and defective graphene and carbon nanotubes. This result is consistent with previous observations that carbon nanotubes and graphene act as electron acceptors with respect to COOH groups.

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Nabil Al-Aqtash
New Mexico State University

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