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Ab Initio Study of Carboxylated Graphene[1] NABIL AL-AQTASH, IGOR VASILIEV, New Mexico State UniVersity — We investigate chemical functionalization of graphene by carboxyl (COOH) groups using first principles computational methods. The binding energies and equilibrium geometries of COOH groups covalently attached to graphene clusters with no surface defects, Stone-Wales defects, and vacancies are examined in the framework of density functional theory combined with the generalized gradient approximation. We find that the attachment of COOH groups induces substantial structural changes in graphene. Our calculations show that the binding of the COOH group to graphene is significantly stronger in the presence of surface defects. This result suggest an important role of point surface defects in the carboxylation of graphene.

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