

Abstract Submitted  
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**First-Principles Studies of Covalent Functionalization of Graphene by Carboxyl Groups**<sup>1</sup> NABIL AL-AQTASH, IGOR VASILIEV, Department of Physics, New Mexico State University, Las Cruces, New Mexico — We study the mechanism of covalent functionalization of graphene by the carboxyl (COOH) group in the framework of density functional theory combined with the generalized gradient approximation. The structures and binding energies of the COOH group attached to the surface of graphene are examined in cases of graphene containing no defects, containing a Stone-Wales defect, and containing a vacancy. Our calculations confirm that the binding of the COOH group with graphene is significantly stronger in the presence of surface defects. We also observe substantial changes in the structure of defective graphene after the attachment of the COOH group. These results suggest that surface defects play an important role in the carboxylation of graphene.

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