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Ab Initio Study of Covalent Functionalization of Defective Carbon Nanotubes by Carboxyl Group[1] NABIL AL-AQTASH, IGOR VASILIEV, Department of Physics, New Mexico State University, Las Cruces, New Mexico 88003 — Covalent sidewall functionalization of carbon nanotubes with carboxyl groups (COOH) is investigated using first principles computational methods. The binding energies and equilibrium geometries of functionalized nanotubes with no surface defects, Stone-Wales defects and vacancies are calculated in the framework of density functional theory combined with the generalized gradient approximation. Our calculations show that the binding of COOH groups with carbon nanotubes containing surface defects is stronger than that with defect-free nanotubes. Furthermore, the presence of COOH groups on the surface leads to a considerable change of the electronic and structural properties of defective nanotubes. Our results suggest that surface defects play an important role in the formation of chemical bonds between carboxyl groups and carbon nanotubes.

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