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Role of Surface Defects in the Carboxylation of Carbon Nanotubes: An *Ab Initio* Study[1] NABIL AL AQTASH, IGOR VASILIEV, Department of Physics, New Mexico State University, Las Cruces, New Mexico — We investigate the mechanism of covalent sidewall functionalization of carbon nanotubes with carboxyl groups using first principles computational methods. The binding energies and equilibrium geometries of carboxylated 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 carboxyl groups with carbon nanotubes containing surface defects is stronger than that with defect-free nanotubes. Furthermore, the presence of carboxyl 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 chemical groups and carbon nanotubes.

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