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Ab Initio **Study of Crosslinking of Functionalized Carbon Nanotubes**[1] IGOR VASILIEV, SEAMUS A. CURRAN, Department of Physics, New Mexico State University — We investigate the mechanism of covalent crosslinking between carbon nanotubes functionalized with thiocarboxylic and dithiocarboxylic esters. The structures of interconnected nanotubes are modeled in the framework of density functional theory combined with the pseudopotential approximation. Our calculations reveal an important role of surface defects in the formation of chemical bonds connecting nanotubes to each other. The strength and stability of intertube bonds increases in the vicinity of defect sites. The computed binding energies and potential energy profiles of linked nanotubes are found to be sensitive to the choice of the exchange-correlation functional used within the density functional formalism. This sensitivity could be explained by a nonuniform distribution of the electronic charge density near defect sites. Our results imply that the use of gradient-corrected functionals is essential for accurate theoretical modeling of functionalized carbon nanotubes and nanotube-based composites.

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