Magnetic, mechanical, and adsorption properties of cross-linking carbon nanotubes

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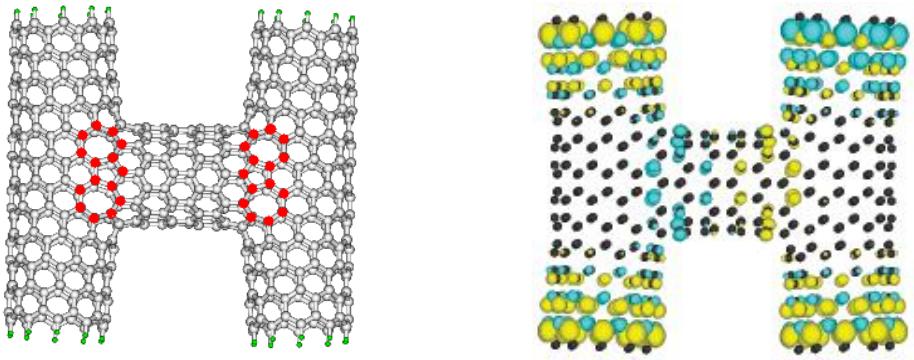
Cross-linking carbon nanotubes (CLCNTs) composed of three axially confined single-walled carbon nanotubes (SWCNTs) of the (10,0) type are investigated by plane-wave density functional theory (DFT). Three CLCNT models, differing from each other by the structure of the contact regions of the three SWCNT constituents, are explored in terms of their geometric, electronic, and magnetic properties. Various magnetic phases, as obtained by combining finite SWCNTs in ferromagnetic (FM) or antiferromagnetic (AFM) coordination, are distinguished. The characteristics of these phases are shown to depend on the contact region geometry which plays an essential role in defining the order of their stabilities. For a selected CLCNT, adsorption of hydrogen atoms is discussed. The magnetic features of the CLCNTs turn out to hold the key for understanding the site dependence of the hydrogen atom adsorption energies. The CLCNT behavior under strain applied along the bridge axis is studied, and a detailed image of CLCNT rupture emerges from observing C-C bond elongation and bond breaking in the contact region.



(a) (b)

Representation of the geometry (a) and the three-dimensional spin density distribution (b) for a CLCNT with adjacent pentagons and heptagons in the contact region.