Magnetism in finite-sized single walled carbon nanotubes of the zigzag type.

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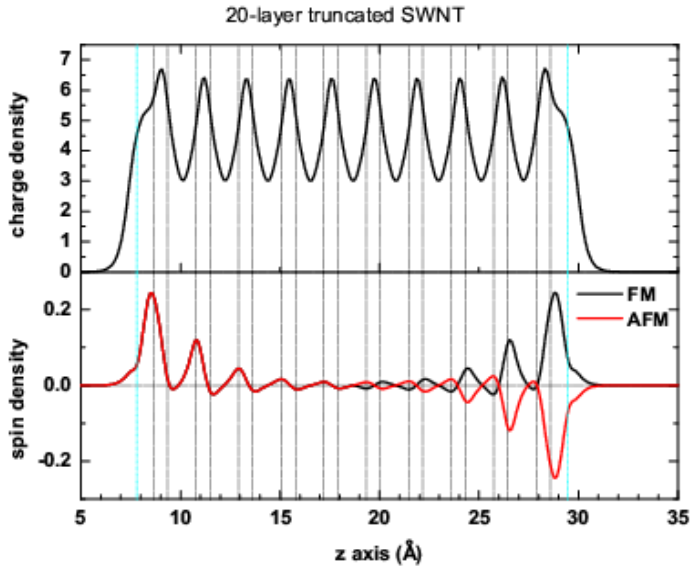
The magnetic properties of (10,0) finite sized single walled carbon nanotubes (SWNTs) are investigated by density functional theory (DFT). In particular, a comparative study on the impact of different nanotube terminating structures on the magnetic states of these systems is presented. Three termination modes are included: hydrogenation, truncation with edge reconstruction, and capping by fullerene hemispheres. Magnetic ground states are reported for all systems considered. The magnetic moments of truncated and hydrogenated systems were found to localize at the SWNT ends, with preference for antiparallel orientation, or antiferromagnetic (AFM) order. Capped systems, in contrast, exhibit a delocalized spin density distribution as well as a tendency towards ferromagnetic (FM) order beyond a critical length. The magnetic phenomena described here are attributed to edge effects associated with the reduction of periodic SWNTs to finite size. The spin densities of the considered SWNTs are investigated as a function of their lengths, and an analogy between the resulting structures and the magnetization induced in a non-metal inserted into an environment with itinerant magnetism is outlined.



Charge and spin densities for a 20 layer H-terminated truncated SWNT where FM and AFM order are distinguished. Allowance has been made for geometric reconstruction of the tube ends .