Charge transfer in Fe-intercalated SWCNT

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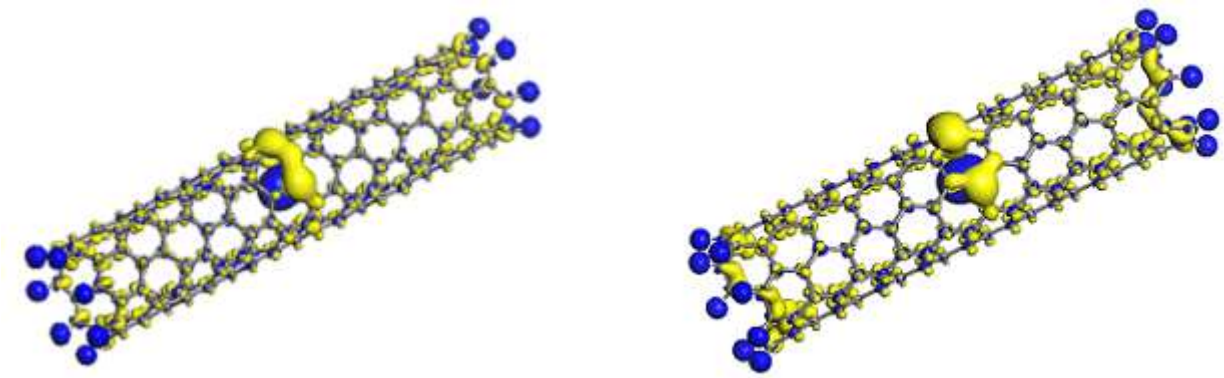

Metal-intercalated nanotubes are perspective materials for nanoelectronics. Up to now, only calculations for nanotubes with alkali metal inclusions were performed. [1, 2, 3] We executed computational simulations of single-wall carbon nanotubes (SWCNT) intercalated by an iron atom. Results of our calculation show, that there is a charge transfer between the iron atom and the nanotube. The nanotube can donate or accept electrons from the iron atom depending on the charge of the whole system. Irrespective to the one of the whole system (taking into account the possible oxidation states of the iron atom, the charges 0, +1, +2, +3 were considered) the charge of the iron atom was in the range of +0.88…+1.08.

No sensitive charge delocalization was found. The negative charge was mainly localized on the two carbon atoms, which are closed to the metal ion. The simulations performed for H-terminated nanotubes showed that the carbon part of the nanotubes was negatively charged even when the charge of the whole system reached +3 (charge of whole NT ≈ +2). So, there seem to be a charge transfer from the hydrogen atoms to the carbon part of the nanotubes.

Similiar results of charge transfer were found for metallic (4.4) and semiconducting (7.0) nanotubes.

Investigations with other metals, nanotubes of other diameters and other terminated atoms are in process.

All calculations were performed by using VAMP, UHF, AM1*.

[1] H. Shimoda, B. Gao, X. P. Tang, A. Kleinhammes, L. Fleming, Y. Wu, O. Zhou, *Phys. Rev. Lett.,* **2002,** *88(1),* 015502
[2] I.V. Zaporotskova, N.G. Lebedev, L.A. Chernozatonskii, *Physics of the Solid State*, **2004,** *46,* 1173
[3] V.G. But'ko, A.A. Gusev, T.N. Shevtsova, Yu.G. Pashkevich, *Low Temp. Phys.,* **2009,** *35(2),* 137