Potential magnetic properties of carbon nanotube fragments (n, 0) with asymmetrical edges

Chernukhina A.A., Ermilov A.Yu.*

Lomonosov Moscow State University, 119991, Moscow, Russia
**e-mail: Sanchik-U@yandex.ru*

Since the very discovery carbon nanotubes attracted interest of scientists thanks to the vast perspectives of their application. According to the concrete ways of rolling up, these structures unexpectedly display a wide variety of properties, including magnetic [1].

The principal aim of this work was to investigate magnetic properties of single-walled carbon nanotube fragments with zigzag-shaped edges (n, 0). In order to compare results of this work and of the main article [2] and to observe regularity of properties, it was suggested to examine finite carbon nanotubes (8, 0) with fragments as long as q = 3, 4, 5. With reference to the main article of comparison a structure with the dehydrogenated zigzag edge (DHZE) at one end and the mono-hydrogenated zigzag edge (MHZE) at the other end was created.

For the electronic structure calculation, we used the same B3LYP functional, basis set 6-31G* as in the article [3]. All the theoretical calculations were performed with PC GAMESS [4]. All the structures were optimized.

Two main schemes of spin coupling were calculated. High-spin scheme (ferromagnetic properties) resulted much lower on the energetic scale than the low--spin variant. Low-spin model correlates with antiferromagnetic properties; in the literature this type of solutions is called the Broken-Symmetry. Furthermore, the energetic differences between the investigated spin states were analyzed.

The results obtained in this work contrast sharply with [2], where LSDA functional was used. An assumption was allowed that such calculation procedure may depend on the type of the exchange-correlation functional. True results can not be yielded using functionals not advanced enough.

Nano-scaled magnetic materials based on suggested structures are extremely promising.

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