Nanocomposites and nanomaterials

Anodes for lithium-ion batteries based on carbon nanotubes: a quantum chemical study

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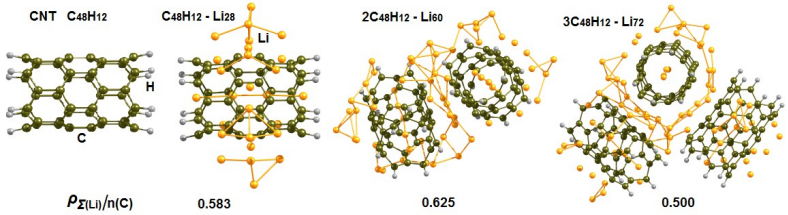
Use of synthetic graphites as anodes in lithium-ion batteries gives no opportunuty to obtain systems with specific capacity of more than 372 mAh/g because of the dominant formation of LiC_6 structures in carbon materials intercalated with lithium. It should be noted that the specific lithium concentration per one carbon atom (ρ) in carbon materials is controlled by their density and porosity. An idea was put forward that rigid carbon matrices – carbon nanotubes (CNT) could be used as carbon source in such systems.

In this work the systems CNT-$Li_{n=0-28}$, 2CNT-$Li_{n=0-60}$, and 3CNT-$Li_{n=0-72}$ have been examined by quantum chemical methods (programsMOPAC 2012 (PM7) and GAMESS). The initial atomic coordinates for calculations of the electronic structure of CNT- Li_n clusters under lithiation were found by molecular mechanics (program HyperChem 7). The structures of CNT and CNT-Li_n nanoclusters a s wellas those of their lithiated forms are shown in the figure.



The results of calculations have shown as follows:

1. In CNT BHT-Li_n systems the elecron density is transferred from the Li_n subcluster onto CNT.
2. The lithium atoms concentration in the CNT-Li_n composites is two or three times greater than that in graphite-like carbon clusters.
3. The volume values of CNT, 2CNT, and 3CNT composites in the processes of lithjiation/delithiation are kept practically (within 0.5-0.8%) the same.
4. CNT's are promising materia for creation of high-capacity anodes for lithium-

ion batteries.