University of zabol
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Faculty of science
Department of chemistry

The Thesis submitted for the Degree of M. Sc
(in the field of physical chemistry)

Title:

Quantum mechanical study of properties of magnesium ion batteries made based on single-walled carbon nanotubes

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Abstract

In this research, initial structures of some armchair single-walled carbon nanotubes were optimized using quantum mechanical computations with M06-2X method and 6-31g(d,p) basis set. Then, interaction of magnesium ion with these structures was studied to evaluate ability of them as magnesium batteries. Results show that formed complexes have good binding energies and carbon nanotubes with larger outer diameters have better binding energies. In fact, increase of diameters of these nanotubes is accompanied by decrease of energy gaps of them and affect on strength of binding to magnesium ion. On the other hand, corresponding boron nitride nanotubes were optimized with similar method and interaction of magnesium ion with these structures was also investigated. Results show that binding energies of complexes of boron nitride nanotubes with magnesium ion are less than those for carbon nanotubes. Furthermore, armchair carbon nanotubes with larger diameters are good choice for designing magnesium ion batteries.

Keywords: Nanotube, Boronnitride, Binding energy, Quantum mechanics