Nanocomposites and nanomaterials

Double-Walled Carbon Nanotubes as a Molecular Container for Anti-Aromatic Systems

O.V. Mykhailenko[1], Yu.I. Prylutskyy[1], I.V. Komarov[1], A.V. Strungar[2], O.O. Mykhailenko[1]

[1] Taras Shevchenko National University of Kyiv, Volodymyrska Str., 64, Kyiv-01601, Ukraine. E-mail: alexm-@ukr.net

[2] Vernadsky National Library of Ukraine, 3, Prospekt Sorokorichchiya Zhovtnya, Kyiv-03039, Ukraine.

Complex compounds of various types and nature have been widely applied in many fields of science and technology. Complex aggregates [1] based on nanostructures such as nanotubes and other compounds, for example, arenes, have unique properties, since a combination of their individual characteristics provides for further growing interest to the research in chemistry, physics, electronics, etc.

There has been theoretically studied a complex of cyclobutadiene with double-walled carbon nanotubes (DWCNT) – (5.5)@(10.10) 270 carbon atoms. The authors have automatically varied the ratio of cyclobutadiene from 4 to 1, with constant concentration of DWCNT. Optical density has been calculated at 350 nm which is recommended by the references for complexes with DWCNT.

Computational data for interaction of cyclobutadiene with DWCNT

(DWCNT/cyclobutadiene)	Absorption, ε	λ (nm)	Δ Absorption
1:0	0,0561	362	
1:1	0,0361	360	0,0200
1:2	0,0321	357	0,0240
1:3	0,0268	352	0,0293
1:4	0,0215	350	0,0346

In the computational spectra there has been observed a slight hypsochromic shift. Absence of solvents and classical molecule functionalisation has proved direct interaction of the molecule-nanocapsule with the host molecule. Such relation of components theoretically enables the creation of complexes of 1:1 and 1:2 types. However, the spectra processing results by the Benesh-Hildebrandt method favour the structure of 1:1 type, and $\boldsymbol{K}_{ass}$ is 99,3 $l \cdot mol^{-1}$ ($\boldsymbol{k}_{корr}$ 0,993).

1. *Mykhailenko O.V., Prylutskyy Y.I., Komarov I.V., Strungar A.V.* Thermodynamic Complexing of Monocyclopentadienylferrum (II) Intercalates with Double-Walled Carbon Nanotubes // Nanoscale Research Letters. – 2016. – Vol.11 – N. 128. – P. 1351-1357.