.Phase transitions in two-layer fullerenes with the non-central effect

Kolesnikova A.[2], Glukhova O.*[1], Kirillova I.[2], Saliy I.[1], Slepchenkov M.[1]

[1]*Department of Physics, Saratov State University, 410012, Saratov, Russia*
[2]*Institute of Nanostructures and Biosystems, Saratov State University, 410012, Saratov, Russia*
**e-mail: glukhovaoe@info.sgu.ru*

The original research technique of the phase transitions in two-layer fullerenes whose mass centers do not coincide has been developed. The hybrid method effectively combining the tight-binding method with the modified molecular dynamics method [1] and the symmetry analysis of the surface topology of the Van der Walls interaction energy of two-layer fullerene shells forms the theoretical basis of the technique.

Nanosystems of $C_{60}@C_{540}$, $C_{80}@C_{540}$, $C_{180}@C_{540}$ with the icosahedral outer shell have been researched. The energy states of the ground state (E_1) and the excited states (E_2, E_3) of the internal fullerene have been calculated. The values of energies E_1, E_2, E_3 and values of formation enthalpy of two-layer fullerenes are represented in the table.

Table

Nanoclusters with the non-central effect	$C_{60}@C_{540}$	$C_{80}@C_{540}$	$C_{180}@C_{540}$
ΔH, $kcal/mol$; $C_m + C_n \rightarrow C_m@C_n$	-2.00	-71.78	-194.23
E_1, eV	-1.972	-2.569	-7.932
E_2, eV	-1.691	-2.288	-7.908
E_3, eV	-1.643	-2.270	-7.907

In the equilibrium state (0 K) C_{60} is localized in one of the 20 potential wells along the axis of fifth-order symmetry of the fullerene C_{540}. The C_{60} molecule began to jump between the potential wells with temperature increase. Thus it is established that nanosystem does not collapse and the hopping frequency of the internal fullerenes between the potential wells increases with temperature rising.

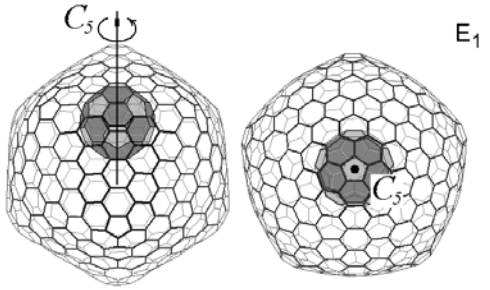

Figure. Molecule C_{60} inside fullerene C_{540}: the ground state.

[1] Glukhova O.E., Saliy I.N., Zhnichkov R.Y., Khvatov I.A., Kolesnikova A.S., Slepchenkov M.M., *J. Phys.: Conf. Ser.* **248**, 012004 (2010).