SELF-STABILITY OF C60@C180 DOUBLE LAYER NANOCAPSULES

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In this work, we used supercomputing parallel processing Quantum Espresso code, and the Electronic Density Functional Theory (DFT) in its Local Density Approximation (LDA), with the Perdew-Burke-Erzerhof (PBE) exchange-correlation norm-conserving pseudo potential. We calculated the optimized configuration of the well-known fullerene C60 containing three radioactive iodine diatomic molecules (3131I2). This system showed instability in presence of calcium, phosphorus and strontium atoms which, when they were adsorbed on the surface, broke the fullerene releasing its content of radioactive iodine. Then, we performed the multi-layer fullerene simulation composed by the fullerene C60, inside the buckyball C180. We found that this system of two concentric carbon spheres has the energy -37.133 KeV at the ground state. This system can store, in the inner sphere C60, the three diatomic molecules of radioactive iodine (3131I2), with energy for the ground-state - 38.956 KeV and can adsorb up to 10 calcium atoms on the outer sphere, C180, surface with a total energy for the ground-state of -49.117 keV. The system thus formed: 3I2@C60 @C180 + 10Ca, is stable and constitutes a good capsule with radioactive content capable of interacting with other molecules with chemical calcium affinity, like crystalline calcium phosphate [Ca10(PO4)6(OH)2], as those occurring in the bones in the form of hydroxyapatite.

Keywords: Buckminsterfullerene, Nanocapsules, Calcium physisorption

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