Nanostructured Surfaces

Effect of Molecular Confinement of C_{60} on the van der Waals Bonding in Clusters of Helium

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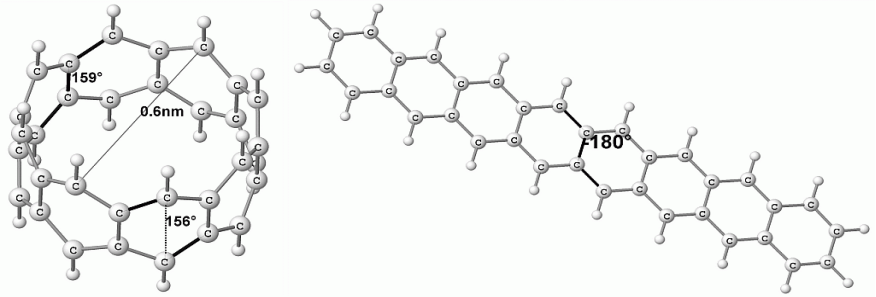
We study encapsulation of van der Waals clusters of helium, He_n, into C_{60}, a typical member of nanosized particles, characterized by a high surface-to-volume ratio. The C_{60}-surface composed of 12 pentagons and 20 hexagons (benzene rings) plays a twofold role: first, it shapes the 'buckled' boundaries of molecular confinement that may encapsulate atom or molecule into its void of a diameter of ~0.71 nm, thus forming an endohedral fullerene, and second, it nests the LUMO, the empty orbital actually functioning as a strong electron hole accommodating maximum 6 electrons.

Two approaches were invoked to study of whether C_{60} confines He_n, thus forming endohedral fullerenes $He_n@C_{60}$: the dispersion-corrected DFT program ORCA and the GAUSSIAN. It is demonstrated that within C_{60}-void, the He atoms are covalently bonded with the bond lengths of 1.941 Å. These cluster-formation is governed by the ionic-model mechanism: C_{60}-surface that confines dopant atoms features a rather strong electron deficiency which is however lower the first ionization energy of He atom. The two molecules built from benzene rings (see Figure) have also been considered in order to demonstrate that buckling



of molecular topology considerably influences properties of benzene rings. The atoms of He while encapsulating into the fullerene's void are subjected to a charge transfer to the C_{60}-surface and thus form the He cluster inside C_{60}.