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Molecular Mechanics and Molecular Dynamics Studies of Complexes of Fullerenes and Carbon Nanotubes

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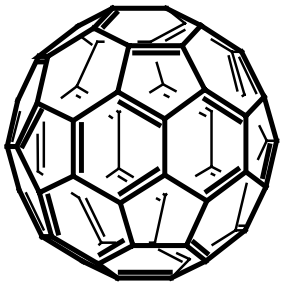

Fullerenes and carbon nanotubes represent an exciting class of molecules. Their hollow structures enable the formation of endohedral complexes with atoms, ions or molecules, with a wide range of potential applications. One of the most fascinating proposed applications involves endohedral fullerene complexes. Buried inside one another, fullerenes can also form nested structures such as $C_{60}@C_{240}$, which are characterized by a high thermal stability. Carbon nanotubes are very promising candidates for industrial applications because of their excellent physical properties (*i.e.* high stiffness, electrical and thermal conductivity, *etc*). For instance, the use of nanotubes as hydrogen storage devices has been proposed. In this talk, we will present the results of molecular mechanics and molecular dynamics calculations for several complexes of fullerenes and nanotubes, paying particular attention to: 1) which guest molecules, being encapsulated, can form stable complexes with fullerenes; 2) which forces drive the formation of nested fullerenes; 3) which outer fullerene cages are most suitable for the stabilization of the unstable inner C_{20} cage; and 4) whether carbon nanotubes may be employed to store molecular hydrogen through physisorption.

Dr. Grygoriy A. Dolgonos received his PhD in Physical Chemistry in 2004 under the direction of Prof. H. Dodziuk at the Institute of Physical Chemistry, Warsaw, Poland for the theoretical investigation of some supramolecular complexes of fullerenes and carbon nanotubes. During his PhD study, he also perfomed calculations of the NMR chemical shifts and spin-spin coupling constants of bicyclobutane (in collaboration with Prof. M. Jaszunski) and of the relative stability of hydrocarbon molecules with unusual spatial structure (in collaboration with Prof. J. Leszczynski). He was also involved in some experimental studies of carbon nanotubes solubilization and of complex formation of camphora enantiomers / dendrimers with cyclodextrins. After completing his PhD, he joined the research group of Dr. Gilles H. Peslherbe at Concordia University as a Postdoctoral Fellow. His current work is focused on the fragmentation of novel fullerene-based materials.