

## The dipole moments of deuterated endofullerenes isotopologues HD@C<sub>60</sub> and HT@C<sub>60</sub>

Antônio F. C. Arapiraca<sup>1,2</sup>, José Rachid Mohallem<sup>2</sup>

<sup>1</sup> *Coordenação de Área de Ciências, CEFET-MG, Belo Horizonte, Minas Gerais*

<sup>2</sup> *Laboratório de Átomos e Moléculas Especiais, Departamento de Física, ICEx, UFMG, Belo Horizonte, Minas Gerais*

The encapsulation of chemical species - atoms, ions or molecules - in nanostructures such as fullerenes and nanotubes has attracted much attention [1], since it has potential applications, for example, in the contexts of medicine and electronics, allowing intelligent drugs and devices to be developed. To understand the charge distributions in these systems is essential for the development of future applications, so the accurate prediction of the electrical properties of these endohedral nanostructures is an important research topic. In addition, modelling the isotopic effect associated with hydrogen substitution by deuterium or tritium may contribute to the description of these systems. In this work we report a theoretical and computational methodology that computes the dipole moments of the deuterated molecular complexes HD@C<sub>60</sub> and HT@C<sub>60</sub>. This approach was used previously to predict the isotopic effect on dipole moments in a variety of apolar and polar molecules [2][3][4]. Here, we observed that the presence of HD and HT induces a polarization in the C<sub>60</sub> cage, causing the dipoles of the complexes to decrease considerably with respect to the dipoles of the isolated molecules. Despite of the lack of the experimental studies to the dipole moment of these systems, this finding is compatible with theoretical [5] and experimental predictions in the literature for the H<sub>2</sub>O@C<sub>60</sub> [6] and HF@C<sub>60</sub> [7] complexes and provides good quantitative insights opening perspectives in the study of the isotopic effect on the dipole moments of deuterated endohedral systems.

**Key-words:** Endohedral fullerenes, dipole moments, isotopic effects

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**References:**

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