Electric-dipole properties of spatially confined water molecule

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Since the recent experimental work of Kurotobi and Murata [1], who demonstrated the so-called molecular surgery approach for the isolation of a C_{60} fullerene containing a single trapped H_2O molecule, the properties of spatially limited water are intensively studied. Particularly interesting is the change in the dipole moment of H_2O upon encapsulation in the fullerene cavity. Theoretical reports regarding to this topic lead to rather opposite conclusions, indicating that the dipole moment value of the $H_2O@C_{60}$ complex is significantly smaller [2,3], slightly bigger [4] or almost equal to that of an isolated H_2O molecule [1].

In this study the confinement-induced changes in the dipole moment of water have been reinvestigated. Additionally, the effect of the orbital compression on the polarizability (α) and first hyperpolarizability (β) was also analyzed. In order to render the influence of the spatial confinement on the properties in question two model spherical confining potentials, mimicking a topology of fullerene cage, were considered. The magnitudes of relevant components of μ, α and β were computed within the finite field method (FF). The calculations have been performed using a wide range of *ab initio* techniques, including Hartree-Fock approximation (HF), the second-order Møller-Plesset perturbation theory (MP2), as well as the coupled-cluster (CCSD and CCSD(T)) methods. Our results demonstrate that depending on the nature of the applied confining potential predicted changes in the analyzed electric-dipole properties differ.

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