Diatomic molecules encaged in fullerene C_{60}: a high-level exploration of their energetic, structural and vibrational properties

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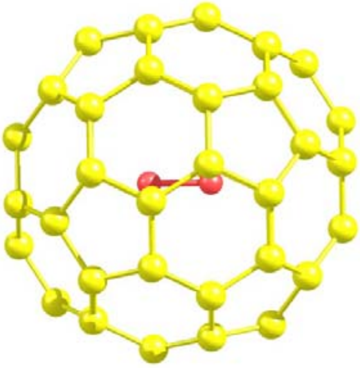

The possibility to encapsulate guest molecules into the cavity of a fullerene (such as C_{60}) is one of the most outstanding properties of this allotropic form of carbon. Many endohedral complexes involving H_2, N_2, H_2O and NH_3 guests with C_{60} have been successfully synthesized via so-called 'molecular surgery' approach (see, for instance, Table 1 of Ref. [1]). However, there is still a lack of accurate computational studies for such endohedral complexes as the large number of atoms to be considered precludes the usage of post-Hartree-Fock methods for these systems. As early as in 1991, Cioslowski predicted [2] stabilization effects of polar and nonpolar diatomic guests in C_{60} cage based on low-level Hartree-Fock calculations, some of which (i.e., harmonic frequency shifts) were not confirmed experimentally. We recently demonstrated [3] that the results of more advanced density-fitting local second-order Møller-Plesset (DF-LMP2) calculations with a triple-zeta basis set lead to an excellent agreement of equilibrium geometries, stabilization energies and harmonic frequencies of the $H_2@C_{60}$ complex with some other sophisticated theories and with experiment.

In the present study, we concentrate on the encapsulation effects associated with the formation of complexes consisting of C_{60} host and diatomic guest molecules by means of (DF-L)MP2 theory. The guest molecules studied include homonuclear (N_2, O_2) as well as heteronuclear (HF, CO, LiH, LiF) species. Stabilization energies, changes in equilibrium bond lengths and harmonic frequencies will be presented and discussed.

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