Structure and properties of Helium atoms inside fullerenes

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Atoms and molecules confined inside fullerenes exhibit unusual quantum properties of interest to physicists and chemists. We have explored the effects of the confinement on the electronic and nuclear structure of the guest species.

We performed nuclear Hartree-Fock and Full-CI studies for two He_3 atoms confined in $C_{60.}$ The helium atoms are treated as dressed nuclei interacting with each other and with the walls of C_{60} through effective potentials. Our calculations reveal that the He atoms inside the C_{60} cavity are completely delocalized and that nuclear spin statistics plays an important role in the structure and stability of these complexes.