A Quantum Description of the State of ^3He_n Atoms Confined in C_{60} (n=1,2)

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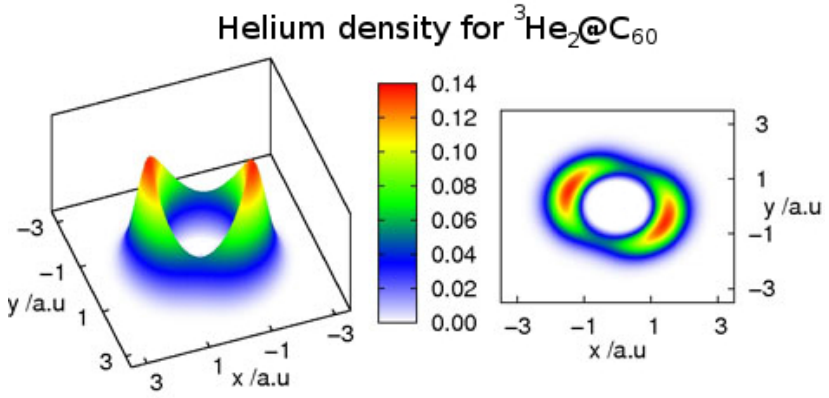
Nuclear wave functions and energies for one and two ^{3}He atoms trapped in Buckminsterfullerene (C_{60}) have been obtained variationally with an approach similar to that used to solve the electronic structure of atoms. Taking into account the fermionic nature of the ^{3}He nucleus we have approximated its nuclear wave function in terms of a Slater determinant. All calculations were performed with a modified version of the recently developed LOWDIN code. To simplify integral evaluation, all potentials and nuclear orbitals were expanded in terms of gaussian type functions. Our results for ^{3}He@C_{60} wave function and energy are in excellent agreement with DVR results. As to the $^3He_2$@C_{60} system, energies and nuclear densities vary dramatically depending of the initial wave function employed in the calculations. Our results show that contrary to intution the ground state of the system correspond to a $|1s1p\rangle$ triplet state configuration. Average distance and energies of this configuration are similar to those obtained via conventional electronic structure calculations. However, our results reveal that the helium atoms are delocalized inside the fullerene.



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