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Quantum Molecular Dynamics Simulation of an Atom Encapsulation by Fullerene

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We have implemented a computer code to perform quantum molecular dynamics (QMD) simulation. The motion of nuclei are treated with Newton's 2nd law of motion; whereas the electrons are treated quantum mechanically using Hartree-Fock approximation. The code has been applied to study how an atom is encapsulated by fullerene (C60). A helium atom is placed 3 Angstrom away from the C60 cage. An initial kinetic energy is then given to the atom, shooting it into the cage. If the initial speed is small, the atom bounces back. By increasing the initial velocity, we can determine the minimum energy required to push the atom inside the C60 cage. QMD is a part a larger set of capabilities in Siam Quantum program.

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