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Quantum Molecular Dynamics Simulation of Lithium Ion in Water Cluster

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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 a small cluster of water molecules, consisting of 28 H2O. The simulated radial distribution function is then compared to the experimental results. A lithium ion is placed adjacent to the water cluster; and an external electric field is applied in order to study how the ion interacts with its surrounding as the ion is accelerated by the external field, and moving through the water molecules. By tracking the speed of the ion, we can determine the mobility of the ion. QMD is a part a larger set of capabilities in Siam Quantum program.

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