Lennard-Jones Potential Determination Via the Time-Dependent Schrödinger Equation

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Abstract

The accurate atomic potential determination is an essential task in the molecular simulations, e.g. Grand Canonical Monte Carlo (GCMC). The ab initio simulations using the quantum mechanics would of great interest in the computational physical chemistry. The numerical simulation of the adsorption phenomenon requires knowing the interactions parameters between the atoms that make up the systems and it sustains the potential to be exploited either. In the present communication, the determination of the interaction parameters for molecular simulation purposes have been extracted by means of solving the Schrödinger equation using finite element method. The PDE implementation of the time-dependent Schrödinger has been successfully achieved through using COMSOL Multiphysics® software. The numerical outcomes give rise the potential curves. By taking advantage of these curves, the appropriate potential parameters have been determined. The effect of temperature and distance has been studied using different interaction potentials for the hydrogen herein.

Figures used in the abstract

Figure 1

Figure 2

Figure 3

Figure 4