

Quantum Chemistry

Seminar 8

Born-Oppenheimer approximation

Exercise 1 (Shaho)

Let's suppose that the atoms of a diatomic molecule interact via the Lennard-Jones potential, $W(r) = 4\varepsilon[(\sigma/r)^{12} - (\sigma/r)^6]$. Find the values of parameters ε and σ knowing that the equilibrium distance of the two atoms is $r_e = 1\text{\AA}$ (Ångström) and their binding energy is $D_e \equiv -W(r_e) = 1\text{eV}$ (electronvolt).

Exercise 2 (unassigned)

Calculate the Hessian matrix of a diatomic molecule, the atoms of which interact via a potential $W(r)$, in its equilibrium geometry, $\vec{r}_1 = [0,0,0]$ and $\vec{r}_2 = [0,0,r_e]$, and show that the matrix has five zero eigenvalues and one which is non-zero.