

# Quantum Chemistry

## Seminar 8

Born-Oppenheimer approximation

### Exercise 1 (Anila)

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  $\varepsilon$  and  $\sigma$  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.