Computerphysik

SoSe 2016

Problem Set 2 – Deadline: April 28, 2016 – 16:15 – seminar room 267

Problem 1: Argon clusters

A cluster of N argon atoms with positions $\vec{r}_k$ has the internal potential energy

$$W_{\mathrm{C}}(\{\vec{r}_k\}) = \sum_{j<k=1}^{N} W_{\mathrm{LJ}}(|\vec{r}_j - \vec{r}_k|),$$

where $W_{\mathrm{LJ}}(r)$ is the Lennard-Jones potential between two atoms

$$W_{\mathrm{LJ}}(r) = 4\epsilon \left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right),$$

r is the distance between the atom centers, $\epsilon = 0.0104$ eV, and $\sigma = 3.40$ Å. Determine the cluster geometry and energy at equilibrium for $N = 2, 3, 4, 5, 6, \ldots$.

Hint: $V_C(\{\vec{r}_k)$ has infinitely many minima because of the translation $(\vec{r}_j \to \vec{r}_j + \vec{t})$ and rotation $(\vec{r}_j \to R\vec{r}_j)$ symmetries of a rigid solid. You should get rid of these degrees of freedom before doing a numerical minimization.