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Problems for *Physik der Materie III*

Due by April 17, 2019

Series 1: Chemical bonding in solids

1.1 The Madelung constant

Calculate the analytical expression of the Madelung constant for a linear chain of alternating positive and negative ions. Briefly explain the result.

1.2 The Lennard-Jones potential

The interaction between two noble-gas atoms at a distance R from each other can be approximated by the Lennard-Jones potential:

$$U(R) = 4\epsilon \left[\left(\frac{\sigma}{R}\right)^{12} - \left(\frac{\sigma}{R}\right)^{6} \right]$$

1) Calculate the distance R_o and the energy $E(R_o)$ at equilibrium ($dU/dR = 0$), as well as the distance R^* where $U = 0$.

2) Using U, determine the energy E_a per atom at equilibrium of an fcc-lattice, where

$$E_a(R) = \frac{1}{2} \sum_{i \neq j} U(R_{ij}).$$

To calculate E_a perform the summation using $R_{ij} = p_{ij} R$ ($R =$ nearest neighbor distance) and the following expressions:

$$\text{a)} \quad \sum_{i \neq j} \left(\frac{1}{p_{ij}}\right)^{12} = 12.13, \qquad \text{b)} \quad \sum_{i \neq j} \left(\frac{1}{p_{ij}}\right)^{6} = 14.45$$

What is the relation between σ and the equilibrium distance R_0' for the fcc lattice ? Compare the result with the one obtained in 1.
Discuss the value of 12.13 considering the atomic arrangement in an fcc lattice.