Phys 771
Condensed Matter Physics
Problem Set # 7

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1. Calculate the ratio of the cohesive energies for Neon in BCC and FCC structures. You need to use the Lennard-Jones potential and the given lattice sums A_6 and A_{12} for both structures as discussed in class. Assume that both structures have the same values of ϵ and σ. Which structure is more stable

2. Use computer to find the lattice sums A_6 and A_{12} for simple cubic lattice.

3. Consider the inert gas crystal of Argon (Ar) which has an FCC structure. The cohesive energy per Ar atom is $\varepsilon/N = 2\ \epsilon\ \{A_{12}(\frac{\sigma}{d})^{12} - A_6(\frac{\sigma}{d})^6\}$, with $\epsilon = 0.0104\ eV$ and $\sigma = 3.4\ \mathring{A}$. Calculate the following quantities at equilibrium; the nearest-neighbor distance d_0, energy per atom ε/N, and Bulk modulus B. Compare the obtained values with those listed in table 11.5 of the textbook

4. Calculate the cohesive energy per one molecule of NaCl and verify that the obtained value is 8.18 eV as given in table 11.8 of textbook. The nearest neighbor distance (d_0) of NaCl and Madelung constant (α) are 2.82 $\mathring{A}$ and 1.747, respectively.

5. Consider a 2D ionic square lattice with nearest-neighbor distance of d as shown in Figure 1. Calculate the first five terms of the electrostatic Coulomb energy (also called Madelung energy) and prove that the obtained Madelung constant is 1.334. Use computer to demonstrate that the accurate value of Madelung constant is 1.6155

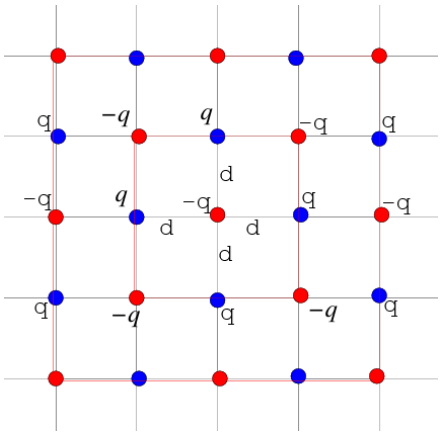

Figure 1: