Háskóli Íslands
Raunvísindadeild
Eðlisfræði

Haust 2015

Eðlisfræði þéttefnis I

Dæmablað 1

Skilafrestur 1. September 2015 kl. 15:00

1. **Ionic crystal KF** (10)

   In a single molecule of KF, the equilibrium internuclear separation is $r_0 = 2.67$ Å and the cohesive energy ($-E_\mathrm{i}$) relative to seperated ions is 0.50 eV/molecule smaller than the Coulomb attractive energy, because of overlap repulsion. Given that the electron affinity of of fluorine is 4.07 eV/electron and that the first ionization potential of potassium is 4.34 volts, show that the energy necessary to separate the molecule into neutral atoms is $-0.945E_\mathrm{i}$.

2. **Cohesive energy of bcc and fcc neon** (15)

   Using the Leonard-Jones potential, calculate the ratio of the cohesive energies of neon in the bcc and fcc structures. The lattice sums for the bcc structures are

   $$\sum_j p_{ij}^{-12} = 9.11418 \quad \text{og} \quad \sum_j p_{ij}^{-6} = 12.2533$$

   and for the fcc structures

   $$\sum_j p_{ij}^{-12} = 12.13188 \quad \text{og} \quad \sum_j p_{ij}^{-6} = 14.45392$$