

Eðlisfræði þéttfnis I

Dæmablað 1

Skilafrestur 29. August 2017 kl. 15:00

1. Ionic Bond Energy Budget (10)

The ionization energy of a sodium atom is about 5.14 eV. The electron affinity of a chlorine atom is about 3.62 eV. When a single sodium atom bonds with a single chlorine atom, the bond length is roughly 0.236 nm. Assuming that the cohesive energy is purely Coulomb energy, calculate the total energy released when a sodium atom and a chlorine atom come together to form a NaCl molecule. Compare your result to the experimental value of 4.26 eV. Qualitatively account for the sign of your error.

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

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

and for the fcc structures

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

3. Madelung's Rule (15)

Use Madelung's rule to deduce the atomic shell filling configuration of the element tungsten (symbol W) which has atomic number 74. Element 118 has recently been

discovered, and is expected to be a noble gas, i.e., is in group VIII. (No real chemistry tests have been performed on the element yet, as the nucleus decays very quickly.) Assuming that Madelung's rule continues to hold, what should the atomic number be for the next noble gas after this one ?