

1. (5 pts) Normally the calculation of the Madelung constant for a particular crystal structure is very difficult. It involves sums which converge very slowly (you have to evaluate a large number of terms to get close to the correct answer). I considered a simpler, two-dimensional crystal as a problem for the homework, but after adding over a hundred terms on my computer, I still didn't have the Madelung constant accurate to 3 decimal places. So let's make it even simpler than the 2-D problem. Imagine that somehow you forced an ionic crystal to form such that the atoms only extended in *one* dimension (maybe our atoms are trapped in a nanotube, for example). Imagine that the crystal is just a line of alternating + and - ions, each spaced apart by a distance r . Show that the Madelung constant α for this arrangement is just equal to

$$-2 \sum_{n=1}^{\infty} \frac{(-1)^n}{n} = 2 \ln(2).$$

2. (4 pts) If the equilibrium spacing for the ionic crystal in the problem above is equal to 0.288 nm and the exclusion principle repulsion term scales as r^{-9} , what is the potential energy (in eV) of an ion when it is at its equilibrium position?
3. (4 pts) The text claims that at the equilibrium separation r_0 the potential U is a minimum. This is true for classical physics. But in quantum mechanics, the expectation value of $\langle r \rangle$ for the ground state does not have to be at the place where U is a minimum. Why is this so?
4. (4 pts) (a) Do ionic crystals tend to be good electrical insulators or good conductors? (b) Why (c) Do they tend to be transparent or opaque to visible light? (d) Why?
5. (4 pts) (a) Which types of solids tend to be more tightly bound together, ionic or covalent? (b) Which types of solids tend to be more tightly bound together, ionic or van der Waals?
6. (4 pts) Given that the electric field generated by a dipole drops off roughly as $1/r^3$, how should the van der Waals force between two polar molecules drop off as r increases (i.e. by what power of r - and note that I asked about *force*, not potential energy).
7. (5 pts) Given that an electric field will induce a dipole moment in a non-polar molecule which is proportional to the field, how should the van der Waals force between one polar and one non-polar molecule drop off as r increases?

Extra problems I recommend you work (not to be turned in)

- If you have access to a computer, calculate the Madelung constant for a 2-D grid of ions in which each ion has 4 nearest neighbors which have the opposite charge (i.e., a + ion has four nearest neighbors which are all - ions).
- Show that the van der Waals force between two non-polar molecules drops off at the same rate as if one of them were polar.