MATRL 218/CHEM277: Assignment 5

Ram Seshadri (seshadri@mrl.ucsb.edu)

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1. For the Lennard-Jones potential:

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

   Determine by setting $\partial U(r)/\partial r = 0$, the value of r/σ for which the potential is minimum.

2. Why do you expect the dispersion (van der Waals) attraction between larger noble gas atoms to be larger than for smaller ones.

3. Can a solid be held together purely through electrostatics ? Consider the equation for the lattice energy, and use this to show that electrostatics (the Coulombic attraction between unlike charges) does not lead to a stable lattice and that the (Pauli) repulsion between the electron cores is essential.

4. Sketch two interpenetrating square lattices, whose origins are separated by $(0.5, 0.5)$, and assign atoms at the corners of the two lattices with opposite charges (a "2D CsCl"). Verify that in the absence of a core repulsion, that these two lattices will merge into one-another.

5. Can you write out the first few terms of the geometric Madelung constant for the above lattice. Does it look like you can sum it up to ∞.

6. Determine the Madelung constant for a 1D lattice of opposite charges. What is the advantage that pairs of opposite charges ("molecules") have in forming a alternating 1D chain. What about their forming rock-salt (use the listed Madelung constants from your notes).

7. Sketch the E *vs.* k dispersion relation for a square lattice of p_x and p_y orbitals, and pay attention to σ and π interactions. The points defining the Brillouin zone boundaries are $\Gamma(0, 0)$, $X(\pi/a, 0)$, $Y(0, \pi/a)$, and $M(\pi/a, \pi/a)$. Sketch the densities of state alongside.

8. Now stretch the above the lattice in the y direction so that it is rectangular, with $a < b$. How does this modify the band structure. Remember that the BZ boundaries are $\Gamma(0, 0)$, $X(\pi/a, 0)$, $Y(0, \pi/b)$, and $M(\pi/a, \pi/b)$. Show that if there is one electron per orbital, such a distortion can result in a gap between filled and unfilled states.