

MATRL 218/CHEM277: Assignment 5**Ram Seshadri (seshadri@mrl.ucsb.edu)****Due date: February 21st 2013**

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. 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"). 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 ∞ .
4. Determine the Madelung constant for a 1D lattice of opposite charges.
5. 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.
6. 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.