MATRL 218: Assignment 3

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1. Use the American Mineralogist database linked on the website to download the crystal structures (as a `.cif` file) of perovskite (the mineral $CaTiO_3$ and sketch the structure using VESTA. Use VESTA to determine all of the distances between Ca and O and between Ti and O. How many near-neighbors do you think Ca has.

2. The Lennard-Jones potential for a monoatomic system is:

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

   Where ϵ is the well depth and σ is the atomic (or particle) diameter. (i) Sketch the distance-dependence of this potential using scaled units, *ie.* set $\sigma = 1$ and $\epsilon = 1$. Approximately how many atomic diameters does one need to be separated by, before there is effectively no interaction. (ii) Determine by setting $\partial U(r)/\partial r = 0$, the value of r/σ for which the potential is minimum.

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

4. Calculate the geometric Madelung potential *per* pair of ions of unit positive and negative charge, separated by unit distance. Now do this for a square (two pairs of ions) and a cube (4 pairs). Do you see convergence to the Rock Salt value of 1.74756? [Bonus question: Write a code that can do this for cubes with increasing edge length and determine how many ion pairs are required to reach the above value.]

5. 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 ∞.

6. Sketch the E *vs.* k dispersion relation for a linear chain (cell parameter a) of p_x orbitals, where the propagating chain runs along x. On the same diagram, sketch the dispersion relation for a chain of p_z orbitals (that point perpendicular to the chain direction).