MATRL 218/CHEM 227: Assignment 1

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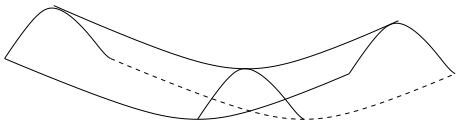
1. Water and silicon share a common feature in that when they melt, their densities increase (at least at 1 bar pressure). Provide a simple structural reason.Do you expect the same behavior from cubic-close packed (fcc) Cu metal.

2. What is the Kauzmann paradox ? Why does the entropy of a liquid decrease when it becomes a glass even though the effective structures of liquids and glasses ("snapshots") are similar.

3. Many liquids can be rapidly quenched to give a glass. Why can't this be indicated in a phase diagram ?

4. It is not possible to tile a flat surface with only pentagons. What if the surface were curved (such as a sphere) ? Can you close-pack disks on the surface of a sphere ? What about the surface of a saddle (see figure)



5. We have discussed two classes of glass structures — crn and rcp. Give examples of glasses which correspond to these. How is one structure expressed in terms of another ?

6. SiO_2 is a glass former whereas PbO is a glass modifier. What do these terms mean structurally ? Why is PbO added to Na_2O/SiO_2 glass ? to make "crystal" ? (The State California now requires such lead crystal to carry a warning).

7. Why is the crystallization of hard spheres, with no attractive interaction between them, considered to be entropy stabilized ? See the reference by Lekkerkerer in your notes.

8. See this paper by David Norris *Adv. Mater.* **16** (2004) p 1393 [DOI link] and explain how the flow of the carrier liquid can affect the crystal structure formed by hard colloidal spheres.

9. Calculate the geometric Madelung potential on a cation that forms a part of a 1D chain, if it's nearest neighbors are anions at a distance of 1, second nearest neighbors are cations at a distance 2, third nearest neighbors are anions at a distance 4 and so on. Assume magnitudes of the charges = 1.

10. The Buckingham potential between like atoms can be written:

$$U(r) = A\exp(\frac{-r}{\sigma}) - C(\frac{\sigma}{r})^6$$

What is the equilibrium separation between two atoms that obey such an attractive potential, and what is the energy by which the atoms are stabilized when they come together from ∞. A and C are parameters, and σ is the diameter of the atom.