

## Homework assignment #4 for CCB 422/522, Spring 2021

*Please show your work for all problems!*

1. Consider a uniformly charged spherical volume with radius  $R$  and space charge density  $\rho$  (*i.e.* in units of charge/volume). What is the electric field for  $r < R$  and for  $r > R$ ? *Hint:* use Gauss' law where the surface is the surface of a sphere of radius  $r$ .
2. (*Harder*). Consider the same spherical volume as in problem 1, but now solve Poisson's equation to determine  $\phi(r)$  as a function of  $r$ .
3. Consider a cluster formed (in the gas phase) of a single  $\text{Na}^+$  ion surrounded by 6 nearest neighbor  $\text{Cl}^-$  ions, arranged in an octahedron; cf. Example 20-3 in your text. Is this cluster stable, relative to the seven ions infinitely far apart? (It is not enough to say "yes" or "no"! You must show your work.)
4. As an estimate for the free energy of burying a charged amino acid such as aspartic or glutamic acid in protein folding, compute the free energy (in kcal/mol) of transferring an ion of radius  $3 \text{ \AA}$  and charge  $+1$  from water to oil. Assume that water has a dielectric constant  $\epsilon_w = 80$ , and oil has  $\epsilon_{oil} = 2$ .
5. What is the free energy cost (in kcal/mol) of transferring a monovalent anion of radius  $a = 2 \text{ \AA}$  and a monovalent cation of the same radius  $a$  from water ( $\epsilon = 80$ ) into oil ( $\epsilon = 2$ ) at an ion-paired separation of  $2a = 4 \text{ \AA}$ ?