Project #2 – Chem 537

Project Proposal (1/2 page and a few refs for Aurora approval): **due Friday April 8**
Report Due: Friday May 7
Class Presentation: Wed May 4 (or TBD based upon finals schedule)

Goal: to identify a small series of MD or MC or combination of MD/MC experiments associated with a topic that has a clearly identify a stated scientific need for knowledge and where molecular simulation could be used to address a hypothesis or need for knowledge. You must provide at least 1 (preferably more) references that justify the goal as well as the approach taken.

Computational Protocol:

a) You may use MD, MC or a combination of MD/MC to achieve the stated goal. You may choose the software of your preference.
b) The force fields employed must be justified – however you do not need to choose different force fields and test them.
c) You will need to benchmark your computational protocol to at least 1 but preferably more experimental data (e.g. RDFs or diffusion coefficients) and prove that you are in "equilibrium" if you are doing an equilibrium simulation. If you are not doing an equilibrium simulation, you will need to benchmark against an appropriate time correlation function.
d) Once you have your equilibrium ensemble you will need to justify and describe the analyses performed – which is key to the goal of what you are trying to learn. For example, if your trying to understand how the structure of an electrolyte solution changes as a function of concentration, then you would analyze the RDF's and develop other analyses to try to identify contact ion pairs and solvent separated ion pairs.

Project Report:

a) A 1 page background introduction that clearly identifies the scientific question and its context. What you will learn from your simulations that addresses the scientific question.
b) 2-3 pages of computational methods. This includes the computational protocol, but also any review of how the methodology works…particularly if there are unique aspects to the methodology that are relevant (for example, if you chose a specific ensemble so that you could calculate specific thermodynamic quantities), or if you used an approach or learned an approach that we did not discuss in class (like thermodynamic integration or potential of mean force simulations). All force fields need to be tabulated, information on the mixing rules, etc.
c) 1 page of benchmarking – demonstrate your system is equilibrated, that your simulation is reproducing some key experimental characteristics, etc.
d) 2-3 pages of results and discussion – this will consist primarily of the analysis of the simulation that teaches you what you were trying to learn. You can add the context

of how this fits in and agrees with prior literature or compares to prior hypotheses or models of the system.

e) References need to be included