

Chem 860. HW1 - Molecular Force Field

Due: Feb. 2

January 24, 2009

1. Think of one example related to your own research for which the standard non-polarizable force field (e.g., CHARMM) may *not* be the proper choice. Discuss why and what modifications are needed.
2. Look into the topology and parameter files in CHARMM/GROMACS (e.g., CHARMM 27 force field for protein and nucleic acids: top_all27_na.rtf and par_all27_prot_na.prm). Follow the format and write a new topology entry for a $\beta^{2,3}$ -Ala residue (one more -CH(CH₃)-group between the amide and carbonyl groups than the natural α amino acid). If we can use parameters for atoms similar to those found in the standard α amino acids, point out what new parameters need to be developed.
3. Get familiar with VMD. Take the pdb file on the course website, display with VMD. Use “CPK” for the small peptide and “lines” for water, take a snapshot to include in your report. *Hint: you can adjust the resolution to make nice plots.* **Extra:** take the psf/dcd files also available from the course website, load into VMD to watch a short molecular dynamics trajectory.
4. Optional for CHARMM users: get familiar with CHARMM-GUI: <http://www.charmm-gui.org/>, which has several useful features that allow you to convert PDB files into CHARMM input. Choose your favorite protein (ideally simple, i.e., single chain), download a PDB file from <http://www.charmm-gui.org/>, then generate a protein structure file (PSF) using the PDB reader at CHARMM:GUI (<http://www.charmm-gui.org/?doc=input/pdbreader>); get familiar with the basic structure of a PSF.