Homework Assignment H4
(Due: Monday, 2009/11/16, 4:00 PM)

H4.1. Covalent bond vibrations. A typical energy of a covalent bond is 150 k_BT and its length is 1.5 Å. Assume that the covalent bond can be described by the Lennard–Jones potential given by:

$$V(r) = \frac{a}{r^{12}} - \frac{b}{r^6}.$$

(a) Using the typical energy of the covalent bond as the depth of the potential and the typical bond length as its equilibrium position, find the parameters a and b.

(b) Do a Taylor expansion around the equilibrium position found in (a) to determine the effective spring constant needed to estimate the frequency of vibration.

H4.2. Kinetics of the β-sheet formation. Consider the free energy of the β-sheet, $F_{opt}(M)$, as a function of the number of residue in the β-sheet, M. The free energy for the β-sheet formation, $F_{opt}(M)$, where M is the number of residues in the β-sheet, as well as the size of the nucleus M^* both depend on the free energy of an internal residue, f_β. The time of β-sheet formation $t_\beta = \tau \times \exp(F^*/k_BT)$ depends on the free energy barrier $F^* = F_{opt}(M^*)$. Assume that the elementary time step τ for β-sheet elongation is $\tau = 1$ ns and the thermal energy at a physiological temperature is $k_BT = 0.6 kcal/mol$.

(a) At a physiological temperatures, the time of β-sheet formation was experimentally found, $t_{A,\beta} = 10$ ms, and the size of the nucleus was determined, $M_A^* = 10$. Calculate the free energy of an internal residue, $f_{A,\beta}$.

(b) The protein B is constructed such that the free energy of an internal residue, $f_{B,\beta} = f_{A,\beta}/2$. Assuming that the edge free energies, Δf_β and U are the same for both proteins, A and B, calculate the nucleus size M_B^* and the time of β-sheet formation $t_{B,\beta}$ of the protein B.

H4.3. Selected Questions on the Study: C. Chothia and J. Janin, "Relative orientation of close-packed beta-pleated sheets in proteins," *Proc. Natl. Acad. Sci. USA* **78**, 4146-4150 (1981).
(*For Honors Undergraduate & Graduate Students*).

(a) Why is there a twist between adjacent strands in a β-sheet and what are typical values of this twist?

(b) When β-sheets pack together, some of the side chains will form external surface, and the other will pack together to stabilize the structure. What do you expect to be common to the amino acids that pack together to stabilize the β-structure?