Physical Chemistry Seminar

Tuesday, February 2, 2010 | **11:00 a.m.** | **Room 1315 Chemistry Building**

Microsecond Simulations of the Detailed Folding/Unfolding of Proteins

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The development of new force fields combined with enhanced sampling methods enable us to calculate detailed stability diagrams of proteins and small RNA molecules as a function of temperature, pressure, and urea concentration. These calculations reveal a complex dependence of protein stability on hydration. The balance between folded and unfolded states can be changed adding co-solvents or changing the system volume. Combined studies of the folding of the TRP-cage protein under various conditions reveal the mechanisms for urea denaturation in which van der Waals interactions (not hydrogen bonding) drives the unfolding.

This work is supported by the National Science Foundation, MCB-0543769.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students may meet with the speaker at 1:15 p.m. in Room 8305f