# Physical Chemistry Seminar

**Tuesday, April 20, 2010** | **11:00 a.m.** | **Room 1315 Chemistry Building**

# Simuations of Protein Aggregation in the Cellular Milieu


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A number of diseases, known as amyloid diseases, are associated with pathological protein folding. Incorrectly or partially folded peptides or proteins can self-assemble into a variety of neurotoxic aggregate species, ranging from small soluble oligomers to amyloid fibrils. I will discuss fully atomic simulations of the early stages of aggregation of the amylin peptide (implicated in Type II diabetes) and of the Abeta peptide (implicated in Alzheimer's disease). I will also introduce a novel off-lattice coarse-grained peptide model that can be used to simulate the entire aggregation process from monomers to fibrils. The effects of beta-sheet propensity and of surfaces on the morphology of the aggregates will be discussed.


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**