McElvain Seminar in Physical Chemistry

Tuesday, April 6, 2010 | **11:00 a.m.** | **Room 1315 Chemistry Building**

Modeling the Self-assembly of Nanostructures

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This talk will describe the self-assembly of nanostructured materials, with emphasis on heterogeneous materials that combine nanoparticles with molecules. The talk begins with a survey of self-assembly modeling approaches that have been applied to the assembly of peptide amphiphiles to make cylindrical micelle structures. Then we discuss materials in which DNA is used to link metal nanoparticles or polymers into aggregates or crystalline materials, where unusual structural and thermodynamic properties arise from the interplay of electrostatics, hydrogen bonding and covalent bonding. This is followed by our recent studies of mechanically induced assembly in rotaxane structures, where we show how the interplay of hydrogen bonding with mechanical forces can lead to metastable state formation that is of relevance to nanomachines.

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