

Physical Chemistry Seminar

Tuesday,
January 28, 2014

11:00 am

Room 1315
Chemistry Building

Multiscale Modeling of Macromolecular Dynamics



Professor Cecilia Clementi

*Department of Chemistry and
Chemical & Biomolecular Engineering
Rice University*

Host: Professor Arun Yethiraj

The understanding of emerging collective behaviors in biomolecular complexes represents a major challenge in modern biophysics. As a first step toward the study of such processes we have applied multi-resolution nonlinear dimensionality reduction and diffusion analysis to obtain reliable low-dimensional representations and models for the dynamics of apparently high-dimensional complex systems such as proteins in a biological environment. We have recently developed a multiscale procedure that use this approach to significantly speed up the sampling of rare event of a complex process such as protein folding.

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

Graduate Students may meet with the speaker at 1:00 p.m. in Room 8335