

Seminar

Fall 2011



THE UNIVERSITY OF
SOUTHERN MISSISSIPPI
SCHOOL OF COMPUTING

Title: Multi-Scale Structures and Dynamics By Computer Simulation Modeling: Bio-Functional Nano-Materials To Medicine

Time & Location:

2:00pm, Friday, September 16, 2011
Tec 205 (Vislab), Bobby Chain Technology Building

Presenter:

R.B. Pandey
Department of Physics and Astronomy
The University of Southern Mississippi

Abstract: Particles, chains, sheets, are some of the basic constitutive units to model a range of physical, chemical, and biological systems. Chains (polymer, protein, DNA), sheets (clay platelets, graphene, tethered membranes), and other specific subunits, e.g., aggregates, micro-gels, etc. can be assembled from particles, the smallest units in the coarse-grained description. In recent years we have been investigating structures and dynamics of proteins, peptides, their scaffolding via self- and directed assembly, and binding to specific targets in designing bio-functionalized nano materials (involving multi-scale approaches). Some of these studies will be presented in this talk.