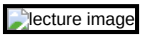

CCT Colloquium Series

Advancing Simulation Methods for Long Time-Scale Chemical and Biological Events

Bin Chen, Assistant Professor
Department of Chemistry, Louisiana State University
Johnston Hall 338
November 10, 2006 - 03:00 pm

Abstract:
Advances in theory and methods have transformed computational science to the extent that computation and modeling are revolutionizing our ways of thinking in every area of science and technology. In particular, realistic, atom-based simulations have significantly improved our capabilities of predicting macroscopic properties and designing novel chemicals and materials with improved functions. Despite their success, computer simulations suffer from severe constraints that reduce the scope of their applications. While the time and spatial scales are limited by the current computer technology and simulation algorithms, our greater understanding of the relationship of biological structure to biological function is bringing new missions and new challenges to molecular simulation. In this talk I will summarize our recent efforts in simulation method development toward the goal of expanding the time-scale accessible to molecular simulation as well as applications of these methods in solving problems of chemical, biological, and environmental interest. Topics to be covered will be selected from:

Speaker's Bio:
Bin Chen received his B.S. in Chemistry with a minor in Computer Science from Peking University, Beijing; his Ph.D. in Chemistry and M.S. in Computer Science from the University of Minnesota, Minneapolis; and Postdoctoral Research at the University of Pennsylvania, Phildelphia. Bin Chen's research is directed toward understanding the relationships between the microscopic structures/interactions and the macroscopic properties for systems of chemical, environmental, and biological interest. The research tool is computer simulation empowered by different levels of theories (from ab initio to classical). Research topics include: development of transferable potentials and efficient algorithms for phase equilibrium calculations; novel computational methods for long time-scale chemical and biological events; vapor

Center for Computation & Technology
2003 Digital Media Center • Telephone: +1 225/578-5890 • Fax: +1 225/578-8957