Physics Colloquium

Michigan Technological University

Friday, March 19, 2010
2:00 pm
Room 101, Fisher Hall

Biomolecular Simulations by Generalized-ensemble Algorithms

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Abstract: Abstract: Protein folding and other biomolecular simulations are very difficult because there exist a huge number of local-minimum energy states and simulations will get trapped in states of such local minima. In order to avoid this difficulty, we employ the so-called generalized-ensemble algorithms, which are based on artificial, non-Boltzmann weight factors and random walks in the potential energy space are realized. From a single simulation run, one can calculate accurate thermodynamic quantities as functions of temperature, etc. Various results of generalized-ensemble simulations of biomolecular systems will be presented.

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