



Forscherguppe 877

Universität Leipzig
Fakultät für Physik und
Geowissenschaften
Institut für Theoretische Physik

Gemeinsames

NTZ - Kolloquium / FOR877-Seminar

Am Donnerstag, dem 05.05.2011 um 17:00 Uhr spricht

Prof. Dr. Y. Okamoto

(Department of Physics, Nagoya University, Japan)

über

Biomolecular simulations by efficient conformational sampling techniques

Conventional computer simulations of biomolecular systems are greatly hampered by the multiple-minima problem, where the simulations tend to get trapped in some of a huge number of local-minimum energy states. In order to overcome this difficulty, we have been advocating the uses of generalized-ensemble algorithms, which are based on non-Boltzmann weight factors. With these algorithms we can explore a wide range of the conformational space. The advantage of generalized-ensemble algorithms such as multicanonical algorithm and replica-exchange method lies in the fact that from only one simulation run, one can obtain accurate estimates of various thermodynamic quantities as functions of temperature. In this talk, I will present some of useful generalized-ensemble algorithms and the latest results of various applications of generalized-ensemble simulations to biomolecular systems.

Ort: ITP, Großer Seminarraum

Interessenten sind herzlich eingeladen!