

Comparison of Sampling Techniques Based on Molecular Dynamics

Jesus A Izaguirre
University of Notre Dame, USA
izaguirr@nd.edu
Molecular dynamics 2

In this talk, I compare sampling techniques based on molecular dynamics, particularly NVT molecular dynamics, replica-exchange umbrella-sampling, and a modification of the latter that uses a highly efficient Shadow Hybrid Monte Carlo method. Both analytical and computational results will be presented on model systems.