



سمینار هفتگی گروه ماده چگال نرم

## Umbrella Sampling Method and Application

Hengameh Shams

Department of Physics  
Sharif University of technology)

To calculate thermodynamic data using a simulation, the system need to be sampled over a sufficient range of configurations. Sometimes ergodicity is hindered by the form of the system's energy landscape. To improve sampling, different techniques are used. One of them is umbrella sampling in which the standard Boltzman weighting for monte carlo sampling is replaced by a potential chosen to cancel the influence of the energy barrier. An alternative to umbrella sampling for computing potentials of mean force is free energy perturbation.

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