

Two Lectures on Molecular Dynamics
by
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Lecture 1:

Molecular Dynamics: an outlook

- Where from MD simulations?
- MD(or, for that, MC) as Equilibrium Statistical Mechanics
- What is an MD simulation?
- Free Energies and Landau Free Energies
- A case study (for progress): rare events

Lecture 2:

Molecular Dynamics: Constraints, restraints and (Landau) free energies

- Two time scales: Holonomic constraints
- Rare Events and Conditional averages: *Blue Moon*
- *Blue Moon* vs Biased (“Non-Boltzmann) Sampling
- A challenging case: Rare Events and Free Energies
 - An application: a simple case of Nucleation