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سمینار هفتگی ماده چگال نرم

## Free energy calculations with non-equilibrium methods: applications of the Jarzynski relationship\*

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Free energies are central quantities to both thermodynamics and kinetics, relating to experimentally determined properties such as equilibrium constants and reaction rates. Even though proper computation of enthalpies is relatively simple at particular molecular conformations, the estimate of the entropic factors requires sampling over large numbers of conformations obeying proper thermodynamic weights. This problem is by no means trivial, and it has been reviewed extensively over the years. Modern applications of free energy calculations in computational chemistry include ligand binding, free energy profiles in mixed quantum-classical enzymatic calculations and hydration. These calculations are done under (if possible) equilibrium conditions, or with as full a sampling as possible. In this seminar we review recent work done using non-equilibrium calculations of free energies, based on the so-called Jarzynski relationship which has been extended and shown to be part of a subset of classical thermodynamics dealing with very small systems, as well as with fluctuations in macroscopic properties.

\* Hui Xiong *et al*, Phys Theor Chem Acc (2006) 116: 338–346

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