سمینار هفتگي ماده چگال نرم

عنوان سمینار

To be in equilibrium, or not to be, that is the question

ارائه دهنده

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چکیده

Calculation of the solvation free energy (SFE) is crucial in many biological processes and geochemical cycles, such as characterisation of protein-ligand binding or exchanging pathway of the persistent organic pollutants between atmosphere and ocean. Here, we introduce a method based on the Hamiltonian adaptive resolution simulation (H-AdResS) to compute the SFE of molecules, using equilibrium statistics and a non-equilibrium identity. In the H-AdResS scheme, solvent molecules are treated concurrently with atomistic and ideal gas resolution according to a generalized Hamiltonian. The two resolutions are coupled through a transition layer in which compensating forces are applied on the molecules within to enforce constant chemical potential throughout the simulation domain. Once an equilibrium uniform density across the resolutions is reached, the molecule/solute is pulled and sampled from atomistic region (solvated state) into ideal gas region (unsolvated state). The pulling process is carried out either in quasi-static equilibrium or in out-of-equilibrium. Using umbrella sampling for the former and Jarzynski's equality for the latter, the resolution-dependent free energy profile is constructed and compared, and subsequently, SFE of the molecule is obtained simply by subtracting the free energies of the two states.

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