

Protein Interactions in Atomistic Studies of Lysozyme Solutions

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A growing point of view about protein interactions focuses on site-distributed interactions between them, which can be relevant both in the crystal [1] and in the disordered phase [2]. As a result of their existence, a specific region of the protein surface interacts with another one, a mechanism underlying protein recognition that can be also depicted in terms of patch-patch interactions [3]. Recently, non-equilibrium molecular dynamics simulations were used to estimate the effective interactions between two lysozyme molecules forming a hydrophobic interface [4]. These atomistic studies with explicit solvent are promising in order to develop accurate, site-distributed models where the degrees of freedom of the solvent and of any electrolyte added to the solution have been averaged out. Such coarse-grained models can be eventually used in computer simulations, which can access longer time and length scales. In fact, the number of atomistic-detailed proteins is limited to one or two molecules, whereas phase transitions are collective phenomena involving many particles [5]. The goal of this presentation is to highlight some aspects of protein interactions by using different methods, namely non-equilibrium molecular dynamics, umbrella sampling and constrained molecular dynamics.

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