Molecular-dynamical model of crystalline lysozyme

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Comprehensive studies of proteins are essential for a variety of challenges faced by humanity nowadays. Modern techniques of decoding protein sequences are now mostly automated and do not require many resources. However, the three-dimensional (3D) structure of a protein is important in addition to its sequence to deeply understand its functions. The x-ray method is considered to be the classical approach to obtaining 3D protein structures. Unfortunately, the crystallization of a protein is needed for it. This can be an issue because of peculiar experimental conditions often necessary for crystallization. Moreover, it is sometimes impossible to crystallize a protein due to its specificuty. Artificial mutations can help, however, they complicate the process as many variations of a protein need to be crystallized. Molecular simulations are used extensively to search for mutations fostering protein crystallization. Furthermore, a molecular-dynamical (MD) model of a crystalline protein can be used to interpret experimental data. An MD model of crystalline lysozyme is created in this work. Neutralization techniques and effects of pH are analyzed [1,2]. The temperature dependence of equilibrium humidity is calculated. Convergence in multiple macroscopic measures is proven. Water mobility is studied. Spatial distribution of mobile water molecules is obtained.

[1] Chresten R S, Mats H O, Michal R and Jan H J 2011 *J. Chem. Theory Comput.* **7** 2284–2295
[2] Mats H O, Chresten R S, Michal R and Jan H J 2011 *J. Chem. Theory Comput.* **7** 525–537