Surf-riding in Thermal Fluctuations of Asymmetric Molecules –

Orientation-dependent Free Diffusion and Directional Transportation of Asymmetrical Molecules at Room Temperature

(Talk #17)

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Tracking of particle diffusion is always considered as a result of the random walk of particles, and thus the displacements of the particle are handled as isotropic. Here, using molecular dynamics (MD) simulations, we show that free diffusion of an asymmetric molecule critically depends on its orientation in a finite timescale of picoseconds to nanoseconds [1]. In a timescale of ~100 ps, there are ~10% more possibilities for the particle moving along the initial orientation than moving opposite to the orientation; and the diffusion distances of the particle reach ~1 nm. We find that the key to this observation is the orientation-dependence of the damping force to the moving of the molecule and a finite time is required to regulate the orientation. Further, we can expect a unidirectional transportation of macroscopic timescale if we constrain the orientation of the asymmetric molecule. This is demonstrated numerically based on a simple theoretical model constituted by a charge dipole (asymmetric charge distribution), where the non-white environmental fluctuation is the key factor [2]. We attribute this unidirectional transportation to the existence of an inherent "equivalent force" along its asymmetric orientation, which drives the asymmetric particle/molecule itself in the environment of fluctuations. "Equivalent force" also exist in the asymmetric molecules in practical systems since thermal fluctuations are not white anymore at nanoscale [3]. MD simulations show that there is unidirectional transportation of a water layer on solid surface at room temperature when the orientations of water molecules have a preference [2].

This finding extends the work of free diffusion to nano-world beyond random Brownian motion, thus will play an essential role in the understanding of the world from a molecular view and the developing of novel technology for various nanoscale and bulk applications, such as chemical separation, water treatment, sensing and drug delivery.

References:

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