Quantifying the Energy Landscape Statistics in Proteins - a Relaxation Mode Analysis ZHIKUN CAI, YANG ZHANG, Univ of Illinois - Urbana
— Energy landscape, the hypersurface in the configurational space, has been a useful concept in describing complex processes that occur over a very long time scale, such as the multistep slow relaxations of supercooled liquids and folding of polypeptide chains into structured proteins. Despite extensive simulation studies, its experimental characterization still remains a challenge. To address this challenge, we developed a relaxation mode analysis (RMA) for liquids under a framework analogous to the normal mode analysis for solids. Using RMA, important statistics of the activation barriers of the energy landscape becomes accessible from experimentally measurable two-point correlation functions, e.g. using quasi-elastic and inelastic scattering experiments. We observed a prominent coarsening effect of the energy landscape. The results were further confirmed by direct sampling of the energy landscape using a metadynamics-like adaptive autonomous basin climbing computation. We first demonstrate RMA in a supercooled liquid when dynamical cooperativity emerges in the landscape-influenced regime. Then we show this framework reveals encouraging energy landscape statistics when applied to proteins.

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