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Title: how does water boost the protein internal motion

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Protein dynamics is crucial for its function and folding, and depends on various external parameters, among which, hydration is of particular importance. Enzymes lose their bio-activity when they are dry and the so-called dynamical transition, manifesting as an anharmonic onset in the mean squared atomic displacement around 180 ~ 230 K, occurs in proteins only when certain hydration level is achieved. Despite decades of study, the microscopic mechanism for how water boosts the protein dynamics and function is still lacking. By combining the neutron scattering and molecular dynamics simulation, the present work decomposes the internal motions of lysozyme on the ps to ns time scales into three components: localized diffusion, methyl group rotation and random jumps. In terms of the energy landscape, the first component is ascribed to be intra-well motion, while the other two correspond to transitions among wells, i.e., barrier-crossing events. The analysis reveals that the major change of protein dynamics on these time scales induced by hydration arises mainly from the intra-well motion ?localized diffusion?, manifesting as increase of the diffusion size, via broadening the well. This result is contradictory to the traditional expectation that the hydration-boosted protein internal motions are barrier-crossing events through lowering the transition barriers, and will make a great impact on the future study of protein dynamics and function.