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"Atomistic Simulation of Single Molecule Experiments: Molecular Machines and a Dynasome Perspective"

Proteins are biological nanomachines which operate at many length and time scales. We combined single molecule, x-ray crystallographic, and cryo-EM data with atomistic simulations to elucidate how these functions are performed at the molecular level. Examples include the mechanics of energy conversion in F-ATP synthase and tRNA translocation within the ribosome. We will further demonstrate how atomistic simulations enable one to mimic, one-to-one, single molecule FRET distance measurements, and thereby to markedly enhance their resolution and accuracy. We will, finally, take a more global view on the 'universe' of protein dynamics motion patterns and demonstrate that a systematic coverage of this 'dynasome' allows one to predict protein function.