Shoot first, ask questions later:
from molecular simulations to protein function

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Proteins carry out an enormous array of functions, from chemical catalysis over molecular sensing to the efficient interconversion of chemical, mechanical, electrical, and light energy. To understand how proteins function, we study their dynamics with molecular simulations that cover a wide range of temporal and spatial scales. At one extreme, we follow fast, photoexcitation-driven protein motions using a hybrid quantum-mechanics/molecular-mechanics (QM/MM) description. The resulting simulation trajectories are compared directly to femtosecond time-resolved protein crystallography and solution scattering experiments at an X-ray free electron laser (XFEL), and to femtosecond optical spectroscopy. At intermediate scales, we study the functional dynamics in molecular rotary motors and pumps using classical molecular dynamics simulations. At the slow extreme, we combine atomistic and coarse-grained simulations to find out how eukaryotic cells probe the physical characteristics of their lipid membranes, and in response activate regulatory processes. For these systems, and for biomolecular machines in general, molecular dynamics simulations provide us with critical insight into the molecular principles underlying their efficient operation.