

Abstract

Evolution provided organisms with a wealth of biomolecules whose promiscuous interactions constitute the "molecular engines" and "gears" propelling life. A staggering array of processes occurs at "nano" temporal and spatial scales remote from our macroscopic intuition. The exponential growth and accessibility of computing power, coupled with continuous refinements in mathematical and physical models of the sub-microscopic scale, are opening up new avenues in the atomistic understanding of protein-protein, protein-drug, self-aggregation, and other biochemical processes. We'll see examples of how "computational microscopes" of increasing reach and sampling power, built through the convergence of engineering, physics and structural biology, are providing new functional insights into the atomistic determinants of biology.