Biomolecular folding and dynamics from single-molecule measurements

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Biological function of proteins and other biomolecules is commonly based on their ability to undergo large conformational changes via activated barrier crossing. Recent single-molecule experiments achieved time resolution sufficient to catch biomolecules in the act of crossing free energy barriers as they fold or undergo other structural changes, offering a window into the elusive reaction "mechanisms". At the same time, molecular simulations have attained timescales where they begin to overlap with single-molecule measurements. These developments put common models and theories of activated barrier crossing to test. In this talk I will describe our recent efforts to understand, using theory, simulations, and experimental information, what happens during the most interesting part of a single-molecule trajectory where it undergoes a large thermal fluctuation allowing it to transition between two distinct conformations (such as the folded and unfolded states).
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