Molecular Machines and Self-Propelled Nanomotors

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Biological systems make frequent use of molecular motors to perform tasks such as active transport of material in the cell, cell locomotion and biochemical synthesis. Proteins, acting as molecular machines, can undergo cyclic internal conformational motions that are coupled to ligand binding and dissociation events. In contrast to their macroscopic counterparts, these nanomachines operate in highly fluctuating environments, which may be crowded by obstacles and other macromolecular species. These environmental factors influence their operation. Recently, a variety of synthetic nanomotors that use chemical reactions to effect self-propulsion have been fabricated. Like their biological counterparts, these nanomotors are subject to strong molecular fluctuations from the environments in which they move. The talk will describe recent work on the simulation of the conformational dynamics of protein machines and directed motion chemically-powered nanomotors. The mechanisms by which these nanomotors and machines operate and some of their possible uses will be described.