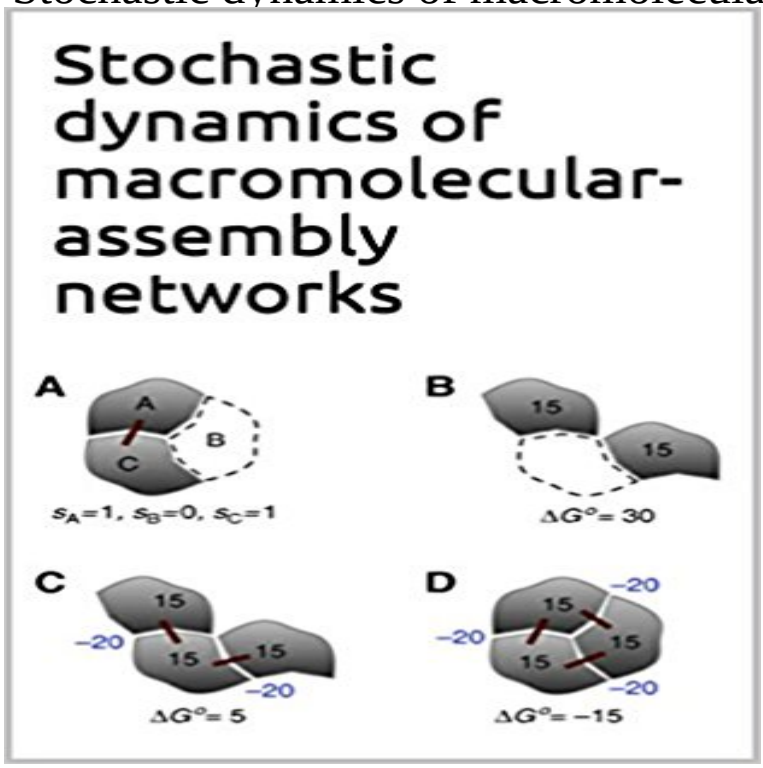
Stochastic dynamics of macromolecular-assembly networks



The formation and regulation of macromolecular complexes provides the backbone of most cellular processes, including gene regulation and signal transduction. The inherent complexity of assembling macromolecular structures makes current computational methods strongly limited for understanding how the physical interactions between cellular components give rise to systemic properties of cells. Here, we present a stochastic approach to study the dynamics of networks formed by macromolecular complexes in terms of the molecular interactions of their components. Exploiting key thermodynamic concepts, this approach makes it possible to both estimate reaction rates and incorporate the resulting assembly dynamics into the stochastic kinetics of cellular networks. As prototype systems, we consider the lac operon and phage ? induction switches, which rely on the formation of DNA loops by proteins and on the integration of these proteinDNA complexes into intracellular networks. This cross-scale approach offers an effective starting point to move forward from network diagrams, such as those of proteinprotein and DNAprotein interaction networks, to the actual dynamics of cellular processes.

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