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Entropy-driven self-assembly of dimers ISSEI NAKAMURA, AN-CHANG SHI, McMaster University — Supramolecular self-assembly is an important phenomenon with applications ranging from chemical synthesis to biological systems. Although the driving force of assembly is the weak non-covalent intermolecular interaction such as hydrogen bonding and dispersion force, the self-assembly is a result from balancing the enthalpic and entropic contributions. In general, the disassembled/disordered phase is expected as temperature is raised because of the entropic gain from the components of the aggregate. However, it has been observed that the self-assembled/ordered phase can be promoted with increasing temperature. This implies that the self-assembly is driven by entropy. In order to provide a better understanding of this entropy-driven transition, we have studied a statistical mechanical model for the aggregation of macromolecular dimers immersed in solvents. The model demonstrates that solvent molecules absorbed on the surface of the solute are released with increasing temperature, leading to an increase of the total entropy of the system. Consequently, the cooperative stability of the dimeric state is induced. The thermodynamic features of this transition are analyzed.

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