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Thermodynamics of protein driven self assembly in membranes RAMAKRISHNAN NATESAN, RICHARD TOURDOT, RYAN BRADLEY, RAVI RADHAKRISHNAN, Unviersity of Pennsylvania — Recent experimental evidences strongly point to the role of proteins and other membrane binding macromolecules in reshaping biological membranes, at length scales of the molecule and the structure enclosed by the membrane. In this work, we investigate the interplay between the membrane curvature induced at the molecular scale, mainly due to peripheral membrane proteins, and the resulting membrane morphologies, of varying complexity, observed at the mesoscale. The biological membrane, in our approach, is represented by a dynamically triangulated surface while the proteins are modeled as curvature fields on the membrane, which can either be isotropic or anisotropic. Thermal undulations in the membrane and cooperativity in the curvature field, due to the stabilization of a nematic phase, drives the membrane into conformations that resembles those in experiments in vivo and vitro. The stability of these structures are examined by two approaches to compute the free energy of the system: (i) Widom insertion technique to compute excess chemical potentials and (ii) thermodynamic integration using the Kirkwood coupling parameter to compute absolute free energies. Building on these methods, we propose a hybrid scheeme that couples both the approaches for computing free energies.

Ramakrishnan Natesan
Unviersity of Pennsylvania

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