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Example

Molecular Dynamics simulations studies of systems capable to floculate in a hydrophobic enviroment: A thermodynamic analysis

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We study the formation of stable incomplete capsids self-assembled from capsomers in solution by means of coarse-grained simulations and an elastic model. We show that during self-assembly, the favorable capsomer-capsomer binding energy competes with the unfavorable stresses generated by the rim of the caps and the elastic stretching due to the spontaneous curvature of the capsid. As a result of that competition, ribbon-shaped and incomplete capsids may emerge as stable structures on very specific conditions. We analyze the conditions required for this process to occur and the influence of the presence of an adsorbing surface in in vitro self-assembly.