

Incomplete capsid formation: coarse-grained and elastic modeling

Carlos I. Mendoza

Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México,
Apdo. Postal 70-360, 04510 México, Cd Mx, Mexico

David Reguera

Departament de Física de la Matèria Condensada, Universitat de Barcelona, Martí i
Franqués 1, 08028 Barcelona, Spain

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.