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Coarse-grained models of key self-assembly processes in HIV-1

JOHN GRIME, The University of Chicago

Computational molecular simulations can elucidate microscopic information that is inaccessible to conventional experimental techniques. However, many processes occur over time and length scales that are beyond the current capabilities of atomic-resolution molecular dynamics (MD). One such process is the self-assembly of the HIV-1 viral capsid, a biological structure that is crucial to viral infectivity. The nucleation and growth of capsid structures requires the interaction of large numbers of capsid proteins within a complicated molecular environment. Coarse-grained (CG) models, where degrees of freedom are removed to produce more computationally efficient models, can in principle access large-scale phenomena such as the nucleation and growth of HIV-1 capsid lattice. We report here studies of the self-assembly behaviors of a CG model of HIV-1 capsid protein, including the influence of the local molecular environment on nucleation and growth processes. Our results suggest a multi-stage process, involving several characteristic structures, eventually producing metastable capsid lattice morphologies that are amenable to subsequent capsid dissociation in order to transmit the viral infection.