Abstract Submitted
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The role of protein interactions in HIV-1 Capsid Shape and Stability: A Multiscale Analysis[1] VINOD KRISHNA, ZHIYONG ZHANG, Dept of Chemistry, University of Utah, WESLEY I. SUNDQUIST, CHRIS P. HILL, Dept of Biochemistry, University of Utah, GREGORY A. VOTH, Dept of Chemistry, University of Utah — A coarse grained model of the HIV-1 CA dimer is constructed based on all-atom molecular dynamics simulations of the C-Terminal capsid dimer. Systematic approaches to identify coarse graining sites within the dimer are presented, and the relationship of the coarse grained model parameters to atomistic properties of the capsid discussed. Coarse grained representations of the capsid shell are constructed and their stability examined. The critical importance of an additional carboxyl-hexameric amino terminal interaction is demonstrated. It is shown that this interaction is responsible for generating the curvature of the capsid shell. It is demonstrated that variation of the strength of this interaction for different proteins in the lattice can cause formation of asymmetric, conical shaped closed capsid shells and it is proposed that variations in the structure of the additional carboxyl-amino terminal binding interface during self assembly are critical to capsid cone formation.

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