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Coarse-grained computational studies of the assembly of viral capsids around a flexible polymer OREN ELRAD, MICHAEL HAGAN, Brandeis University — During the replication of many viruses, hundreds to thousands of protein subunits assemble around the viral nucleic acid to form a protein shell called a capsid. Recent electron microscopy experiments on small ssRNA viruses have shown that their enclosed RNA adopts the icosahedral symmetry of the overall capsid structure. The process that leads to this ordered encapsulation of the RNA is unknown. In this talk, we will explore dynamical simulations of coarse grained models that represent capsid proteins assembling around a flexible polymer, which shed light on the mechanisms by which icosahedral order emerges. We will discuss geometric and kinetic factors that control assembly, including the limits on the length of RNA that can be efficiently packaged. We will also report on several forms of cooperative polymer-protein motions that contribute to efficient and robust assembly. Finally, we will discuss how the simulation predictions can be tested with imaging experiments, bulk assembly kinetics measurements, and recently developed single molecule techniques that monitor the assembly of individual capsids.

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