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How viral capsids adapt to mismatched cargoesidentifying mechanisms of morphology control with simulations[1] OREN ELRAD, 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. Most viruses form one particular structure with astonishing fidelity; yet, recent experiments demonstrate that capsids can assemble with different sizes and morphologies to accommodate nucleic acids or other cargoes such as functionalized nanoparticles. In this talk, we will explore the mechanisms of simultaneous assembly and cargo encapsidation with a computational model that describes the assembly of icosahedral capsids around functionalized nanoparticles. With this model, we find parameter values for which subunits faithfully form empty capsids with a single morphology, but adaptively assemble into different icosahedral morphologies around nanoparticles with different diameters. Analyzing trajectories in which adaptation is or is not successful sheds light on the mechanisms by which capsid morphology may be controlled in vitro and in vivo, and suggests experiments to test these mechanisms. We compare the simulation results to recent experiments in which Brome Mosaic Virus capsid proteins assemble around functionalized nanoparticles, and describe how future experiments can test the model predictions.

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