Dynamical Simulations of Virus Wrapping and Budding

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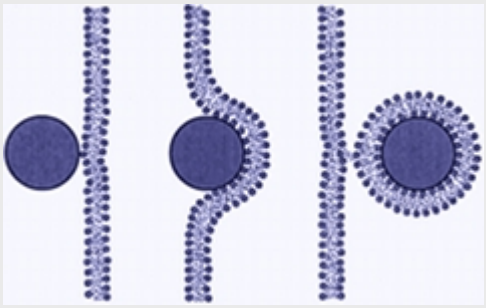

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ABSTRACT:

Enveloped viruses bud through the cell membrane as the final step in their replication process. For many enveloped viruses, a nucleo-protein capsid first assembles in the cytoplasm, attaches to the membrane, and then buds.

We explore this process through modeling the wrapping of a spherical particle by a model bilayer membrane, using coarse-grained molecular dynamics simulations and a theoretical elastic model. Specifically, we study the kinetics and morphologies of wrapping as a function of the relevant system parameters, including the particle radius, the strength of the membrane-particle interaction, and the membrane bending rigidity. The theoretical model predicts a phase diagram as a function of the system parameters, which is compared to results of the dynamics simulations.

Furthermore, the simulations elucidate the dynamical mechanisms by which budding occurs and the structures of intermediate configurations.