Virus self-assembly induced by polyions

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The structural organization of viruses is characterized by simplicity and economy. At a minimal level, the viral genome is composed of either single or double stranded RNA or DNA, surrounded by a spherical-like or cylindrical protein shell composed of many copies of almost identical proteins. The linear size of the virus genome can be tens of microns and is large compared to the diameter of capsid, usually in the range of tens of nanometers, so the genome must undergo a high degree of compaction during viral assembly. *In vivo*, (1) spherical-like viruses with double-stranded genome are made in two steps; first an empty capsid is formed and thereafter the genome is actively transferred into the capsid, whereas (2) spherical-like viruses with single-stranded genome are formed by a co-assembly of capsid subunits and the genome.

During the last decade, spherical-like viruses have been subjected to theoretical modeling using descriptions of different degree of details. Here, we will report on results from molecular dynamic studies of a coarse-grain model describing the process of forming single-stranded viruses possessing icosahedral symmetry. The capsid subunits are represented by rigid, trapezoidal, and charged entities, and the genome by a polyion formed by charged beads connected with harmonic springs. Equilibrium structures were determined, and kinetics of capsid formation was examined by addressing pathways of the co-assembly. The yield of correctly formed capsids depended critically on a balance of the capsomer attraction and the electrostatic interaction. An appreciable lag time appeared before complete capsid formation occurred, in agreement with experimental findings.