493e Understanding Precise Packings in Self-Assembled Convex Structures

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Self-assembly of natural building blocks into unique arrangements with precise packing is ubiquitous in nature and is an intriguing phenomenon. For example, most spherical viruses pack into shells with icosahedral symmetry. Recently progress has been made toward assembly of building blocks into precise and specific structures. Examples include the self-assembly of precision micelles, evaporation driven assembly of colloidal clusters, and superstructures formed via self-assembly of amphiphilic nanoparticles. Elucidating the fundamental physics of these self-assembly processes may provide insights into the origin of precise packing observed in the final structures. Here we combine computer simulation and convex hull searching algorithm to study self-assembly processes. We demonstrate how self-assembly subject to a convex constraint leads to unique polyhedral packing in the self-assembly of cone-shaped particles, colloidal particles suspended in an evaporating droplet, and viral capsomers in icosahedral virus capsids. We also discuss the role of convexity as it pertains to self-assembly as well as the similarities and differences among the precise packings obtained via the previously mentioned self-assembly processes.