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A Precise Packing Sequence for Self-Assembled Convex Structures TING CHEN, ZHENLI ZHANG, SHARON GLOTZER, Department of Chemical Engineering, University of Michigan — We present molecular simulations of the self-assembly of cone-shaped particles with patchy, attractive interactions[1,2]. Upon cooling from random initial conditions, we find that the cones self assemble into clusters and that clusters comprised of particular numbers of cones have a unique and precisely packed structure that is robust over a range of cone angles. These precise clusters form precise packing sequence that for small sizes is identical to that observed in evaporation-driven assembly of colloidal spheres. This sequence is reproduced and extended in simulations of two simple models of spheres self-assembling from random initial conditions subject to convexity constraints, and contains six of the most common virus capsid structures obtained in vivo including large chiral clusters, and a cluster that may correspond to several non- icosahedral, spherical virus capsid structures obtained in vivo. For prolate spheroidal convexity conditions, we demonstrate the formation of several prolate virus structures from self-assembling hard spheres[3].
[1] Chen T, Zhang ZL, Glotzer SC, PNAS, in press (http://xxx.lanl.gov/pdf/cond-mat/ 0608592) [2] Chen T, Zhang ZL, Glotzer SC, http://xxx.lanl.gov/pdf/cond-mat/0608613 [3] Chen T, Glotzer SC http://xxx.lanl.gov/pdf/q-bio.BM/0608040

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