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The role of shape vs. patches in protein crystallization JENS GLASER, SHARON C GLOTZER, Univ of Michigan - Ann Arbor — Proteins fold into a multitude of three-dimensional native structures. The structures of over 100,000 known proteins are deposited in the protein data bank, and most of them have been determined through X-ray crystallography. We ask the question if the role of shape in protein crystallization can be isolated using simulation. Current computational studies show that patchy complementary contacts stabilize experimentally observed P212121 crystal structures for relatively globular protein using spherical protein models. Here we study an anisotropic rigid shape model of green fluorescent protein based on a coarse-grained representation of the atomic coordinates. Using GPU-accelerated molecular dynamics simulations, we find that the experimentally found crystal structure can be stabilized in self-assembly by using complementary attractive patches, confirming the earlier findings. However, we discuss the additional roles of solvent mediated and electrostatic interactions, depletion effects and the self-assembly properties of a purely hard shape model in stabilizing different assemblies. Our findings shed light on fundamental assembly mechanisms in colloidal systems with many competing interactions.

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