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Getting Closer to Real Proteins: Asymmetric and Competing Interactions in Patchy Models[1] PATRICK CHARBONNEAU, DIANA FUSCO, Duke University — Patchy particle models have been proposed to describe protein crystal assembly. Previous analyses of these models typically assume homogeneous patch interactions and symmetric patch geometry, but recent studies suggest otherwise. Typical protein interactions have a wide range of strengths, and sterically competing interactions are the rule rather than the exception. More complex patchy models are thus needed to guide protein crystallization. We study the phase diagram and assembly kinetics of patchy models with varying interaction strength and spatial distribution asymmetry. The results rationalize George and Wilson's observation that proteins with a second virial coefficient within a specific range are easier to crystallize and provide guidelines to facilitate crystallization of recalcitrant proteins. In models with sterically competing patches we also observe distinct crystal forms (dimeric vs. monomeric) depending on the relative strength of the secondary patches.

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