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Self-assembly induced protein crystallization HONGJUN LIU, SANAT KUMAR, Columbia University, JACK DOUGLAS, NIST — The strongly anisotropic nature of inter-protein interactions naturally leads them to self-assemble into structures mirroring the symmetry of the inter-protein potential. Self-assembly is a thermodynamically distinct phenomenon from phase separation, and we consider whether it can play a direct role in nucleating protein crystallization. Previous simulations and measurements have established that protein clusters formed below the critical point for liquid-liquid phase separation (T_c) can facilitate crystal nucleation. However, recent experiments have indicated the existence of clustering-induced protein nucleation even for $T > T_c$, where phase separation does not exist. Here we simulate a minimal model of patchy particles and indeed find that transient clusters formed through self-assembly (even above T_c) can nucleate crystal growth. Importantly, the self-assembled clusters help to select the symmetry of the resulting crystal growth. In contrast, protein crystallization for $T < T_c$ does not have this directing influence, and polycrystalline growth forms, such as spherulites, are then prevalent. Our simulations suggest that self-assembly directed crystallization might be common in protein solutions and that this process is relevant for understanding protein crystallization polymorphism.

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