Abstract Submitted
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Design rules for the self-assembly of a protein crystal[1] STEPHEN WHITELAM, THOMAS HAXTON, Lawrence Berkeley National Lab — Theories and models of protein crystallization based on spheres that form close-packed crystals suggest that protein crystallization can be enhanced by metastable liquid-liquid criticality or demixing, and can be predicted by the osmotic second virial coefficient. However, most protein crystals are open structures, stabilized by anisotropic interactions. I will use analytic theory and computer simulations to argue that the self-assembly of open crystal lattices should not in general be best near the metastable liquid-liquid critical point or binodal (although assembly can certainly happen there), and to argue that the second virial coefficient cannot be a fully predictive measure of assembly propensity (although it is a useful starting point). Instead, the conditions that lead to best self-assembly of one particular computer model of a porous protein crystal are closer to the conditions that lead to best self-assembly of certain model viral capsids than they are to the conditions that optimize assembly of close-packed crystals.

References:
Haxton & Whitelam Soft Matter 2012 & 2013
Whitelam PRL 2010
Whitelam JCP 2010

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