Supplementary Information for “The role of non-specific interactions in a patchy model of protein crystallization”

October 3, 2015

Figure S1: Distribution of symmetry space groups in protein crystals. The most common symmetry space groups of crystals of monomeric proteins, as calculated from a non-redundant set of ~3000 high-resolution protein structures from the Protein Data Bank (http://www.rcsb.org/pdb/home/home.do), accessed in July 2015.
Figure S2: Distribution of unit cell energies and particle volume fractions. Histograms of the energies and particle volume fractions of the sampled $P2_12_12_1$ unit cells, each color representing a different random decoration of patches. Note that, since only the lowest energy structures were of interest, these figures only display data for unit cells with $E_{uc} < -40$ (in units of $\varepsilon_{ns}$).

Figure S3: Poor crystal nucleation for conditions otherwise consistent with crystal growth. Snapshots from the end of simulations with $\eta = 1.0$, $\xi = 3.0$ and (upper image) $\varepsilon_{ns} = 2.0\, kT$ and (lower image) $\varepsilon_{ns} = 2.2\, kT$. Particles colored gray have not created any crystalline bonds. Any other color indicates a crystalline particle.