Supplementary information: Temperature dependence

Average internal energies per particle are calculated in two-dimensional canonical Monte Carlo simulations as:

$$\frac{\langle E^* \rangle}{N} = \langle T^* \rangle + \frac{\langle U^* \rangle}{N} \, , \tag{1}$$

where the first term in the right hand side comes from the kinetic energy contribution, and U^* is the total (sum over particles) reduced potential energy for the system. All of the systems investigated here are finite, in the sense that no periodic boundary conditions are used. In finite-size systems, morphological changes are generally detected with the help of heat capacities per atom, calculated in the canonical ensemble from energy fluctuations, which are directly available during the simulation run. Average reduced heat capacities (where $C_v^* = C_v/k_B$) are given by

$$\frac{\langle C_v^* \rangle}{N} = 1 + \frac{\langle (U^*)^2 \rangle - \langle U^* \rangle^2}{N(T^*)^2} \, . \tag{2}$$

Peaks in the curves of heat capacities as a function of temperature indicate the presence of a change in the morphology of the system. These peaks correspond to inflection points on the curves of average internal energy per particle of equation (1).

The variation of the heat capacity with temperature for racemate B is shown in Figure 1. The rough, strongly fluctuating nature of this plot is indicative of the complex reorganizations taking place in the adsorbed system as the temperature decreases. The heat capacity plot does nevertheless indicate the presence of a high temperature micellization (T^*=3-4) transition. The sharp increase in C_v at low temperatures may be an indication of a freezing transition (T^* <0.1). Snapshots of the configuration of racemate B at T^*=0.05, 0.3, 2.4, and 4.6 are included below, in Figure 2. From the snapshots and the heat capacity plot, the system undergoes a micellization transition around T^*=3. Below this temperature, configurations are dominated by rosette clusters of like molecules.

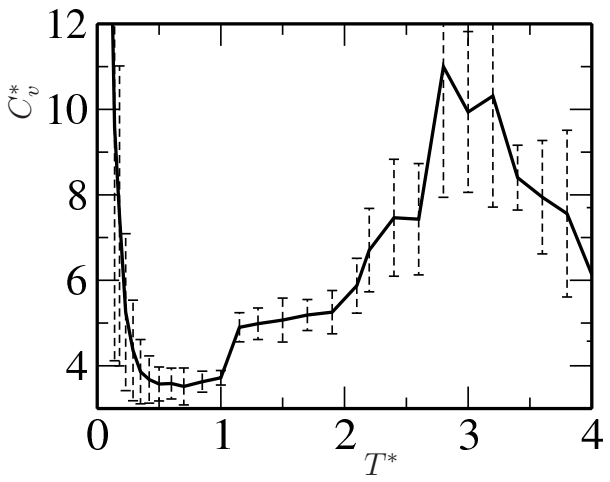

Figure 1: Average heat capacity per molecule for racemate B, as a function of temperature. Fluctuations calculated as standard deviations are indicated by dashed vertical lines. A condensation transition occurs around T^*=3. At low temperatures, the sharp increase in C_v is attributed to a solidification transition.

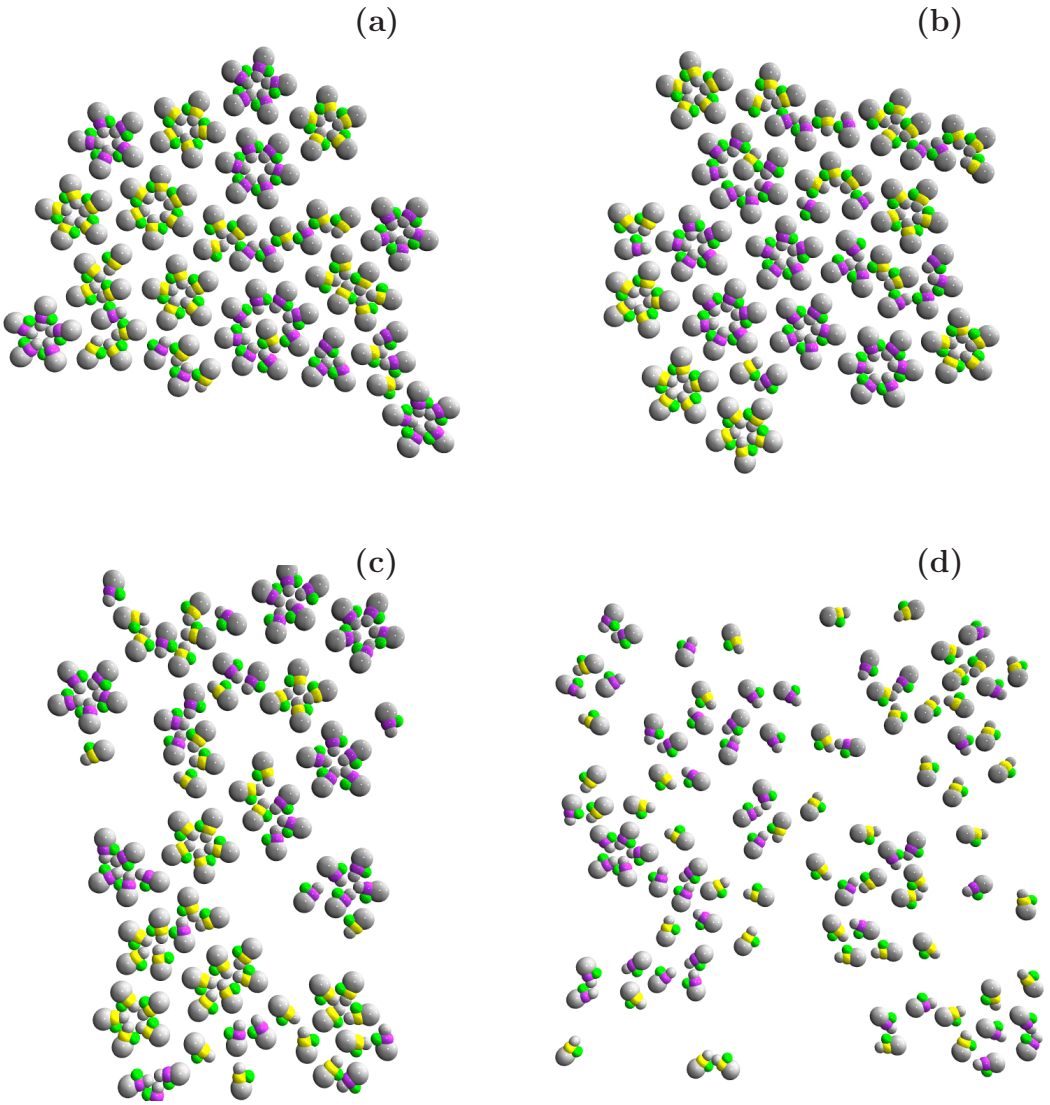

Figure 2: Configurations for racemates of molecule B at T^*=0.05, 0.3, 2.4, and 4.6 (panels (a) through (d), respectively). Although identical, the central atoms in the two enantiomers were indicated in yellow and purple, respectively, for the clarity of the image.