Supporting Information: Thermal Selection of Aqueous Molecular Conformations for Tailored Energetics of Peptide Assemblies at Solid Interfaces

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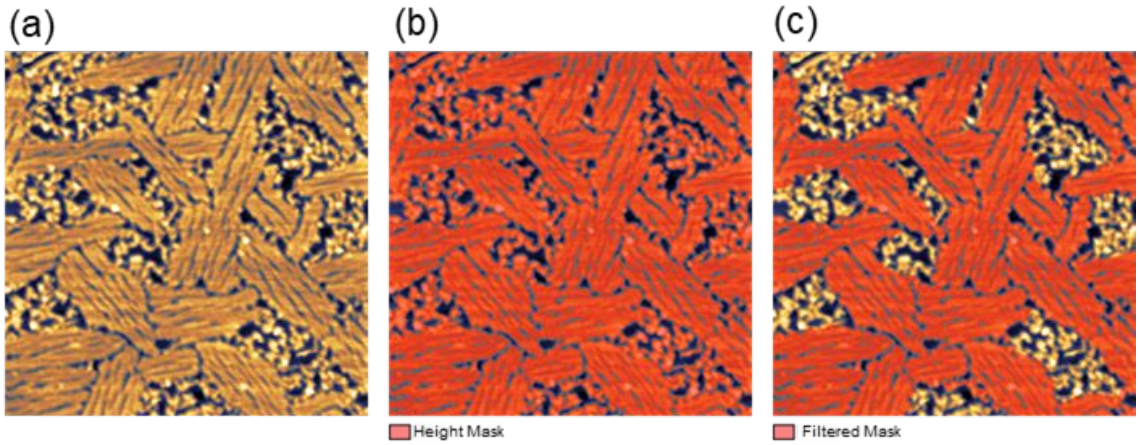
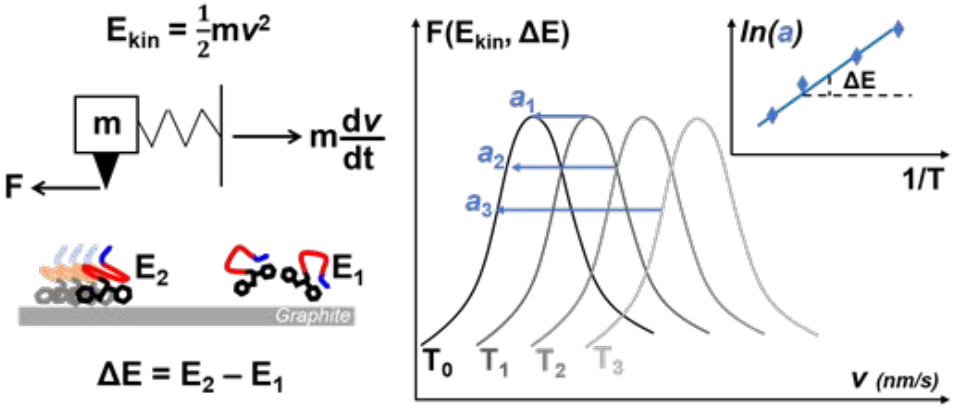
Figure S1: AFM Structural Analysis Technique



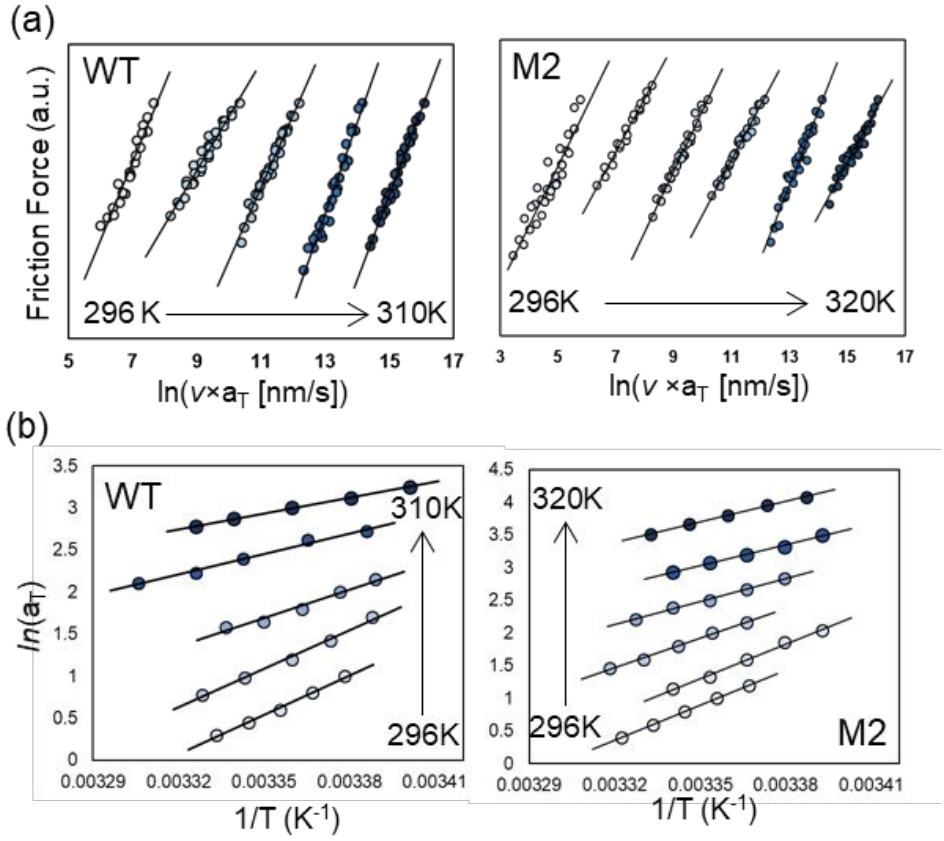
(a) AFM images were processed using the Gwyddion software package.[1] The images are flattened and cropped to remove graphite step edges or other defects that complicate further processing. Phase or amplitude images may be used if defects cannot be cropped from the height image. (b) A mask is applied to flattened image based on height, phase, or amplitude (depending on type of image) so that the peptide is clearly distinguished from the underlying graphite surface. Some additional manual editing of the mask was performed to remove erroneously masked graphite when the computer was unable to automatically exclude it. Moreover, manual editing of the mask was performed when assembled and amorphous peptide structures were erroneously connected as part of the same grain. The mask is then filtered by a variety of grain parameters depending on the quality of the image. In part (c) the mask is filtered by grain size. This was often the most effective at separating the ordered and amorphous regions.

Figure S2: Principle of Intrinsic Friction Analysis (IFA)



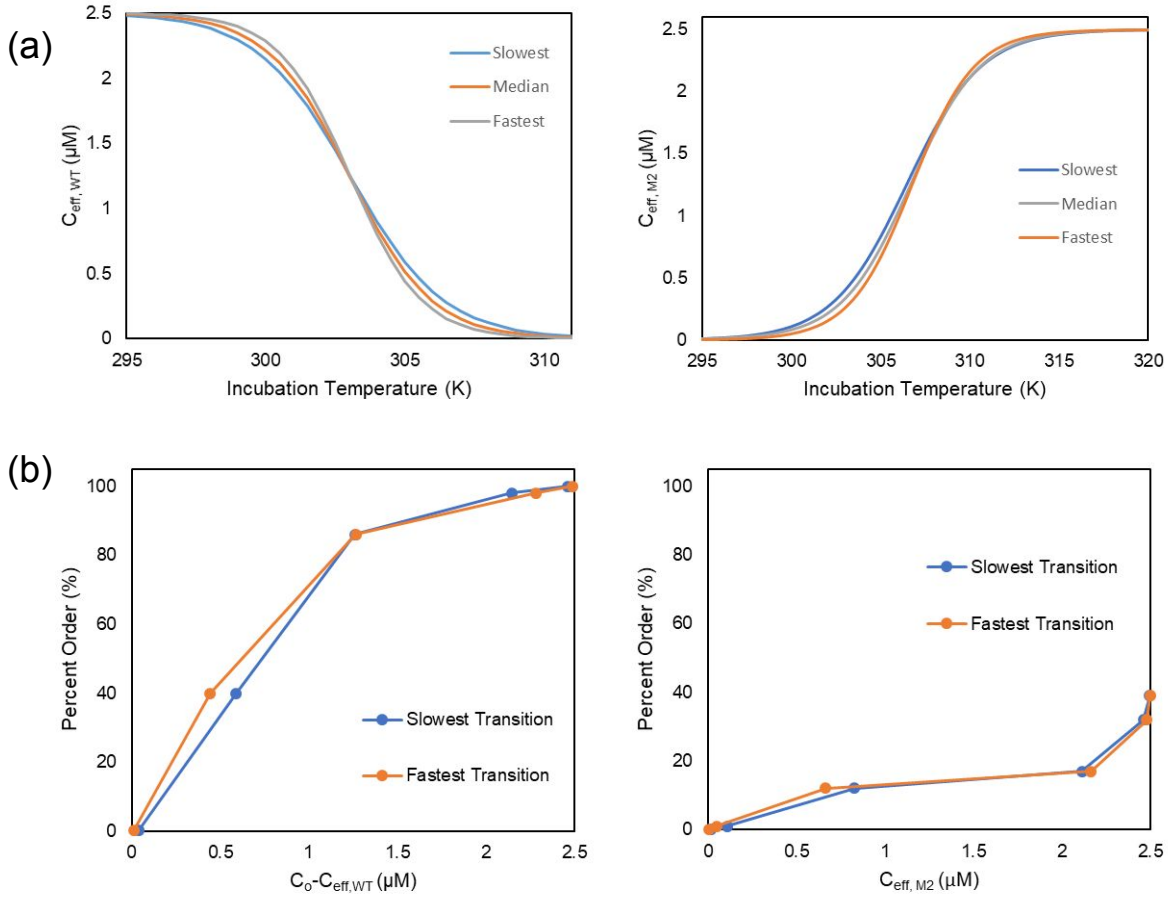
Schematic of lateral forces, F, acting on a SPM tip moving at a scanning velocity, *v*, upon coupling with the structural transition between two peptide energetic states at the surface. Illustration of lateral force spectra obtained at different temperatures and the associated thermal shift factors. The inset is the Arrhenius relationship of the shift factors.

Figure S3: Temperature Dependent Binding Energy of GrBP5-WT and GrBP5-M2



(a) Shifted friction-velocity isotherms for GrBP5-WT (left) and GrBP5-M2 (right) are offset horizontally for clarity. The friction-force intensity has also been scaled and are of arbitrary units. (b) The thermal shift factors, a_T, and the Arrhenius relationship with inverse temperature for data presented in (a) for GrBP5-WT (left) and GrBP5-M2 (right). Arrhenius curves are offset vertically for clarity.

Figure S4: Range of Effective Concentrations estimated from Binding Energy



(a) Plots of the steepest (fastest) and shallowest (slowest) possible sigmoidal dynamics describing the conformational change of GrBP5-WT and GrBP5-M2 with incubation temperature. Propagation of the range of sigmoidal dynamics in (a) was used to determine the range in assembly dynamics, *i.e.,* C_{50} and *k,* were determined from plots in (b). The determined ranges for C_{50}, *k,* T_{50}, and ΔT are tabulated in Table S1.

Table S1: Range of Values for Sigmoidal Fit Parameters

	T_{50} [K]	ΔT [K]	C_{50} [μM]	k [μM^{-1}]
GrBP5-WT	0.01	0.39	0.10	0.23
GrBP5-M2	0.31	0.34	0.05	0.06

Supplementary References

1. Nečas, D.; Klapetek, P., Gwyddion: an open-source software for SPM data analysis. *Open Physics* **2012,** *10* (1), 181-188.