

Supporting Information for

Kinetically Forbidden Transformations of Water

Molecular Assemblies in Hydrophobic Micropores

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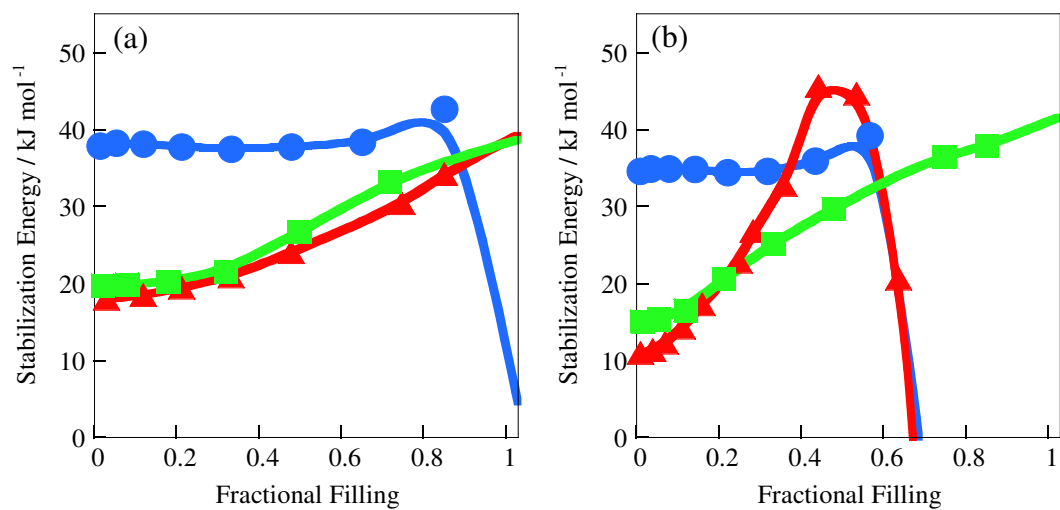


Figure S1. Stabilization energy as a function of fractional filling for $w = 0.5$ (a) and 1.5 nm (b). Clusters: ●, monolayers: ▲, and uniform distribution structure: ■.

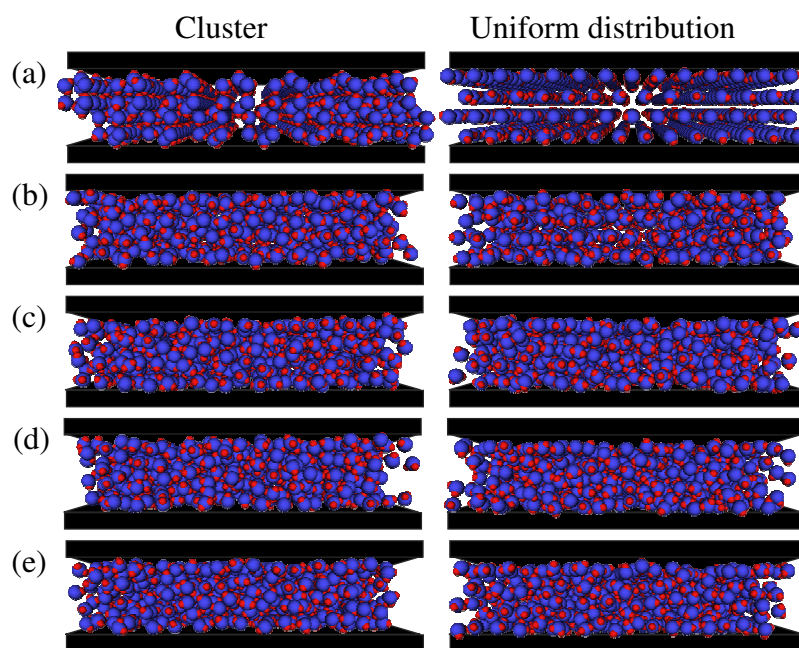


Figure S2. Snapshots showing the cluster–monolayer and uniform distribution structure–monolayer transformations at $\phi = 0.6$ in the micropore of $w = 1.1$ nm, as studied by MD simulation. Time scale = 0 (a), 1 (b), 2 (c), 3 (d), and 4 (e) ps.

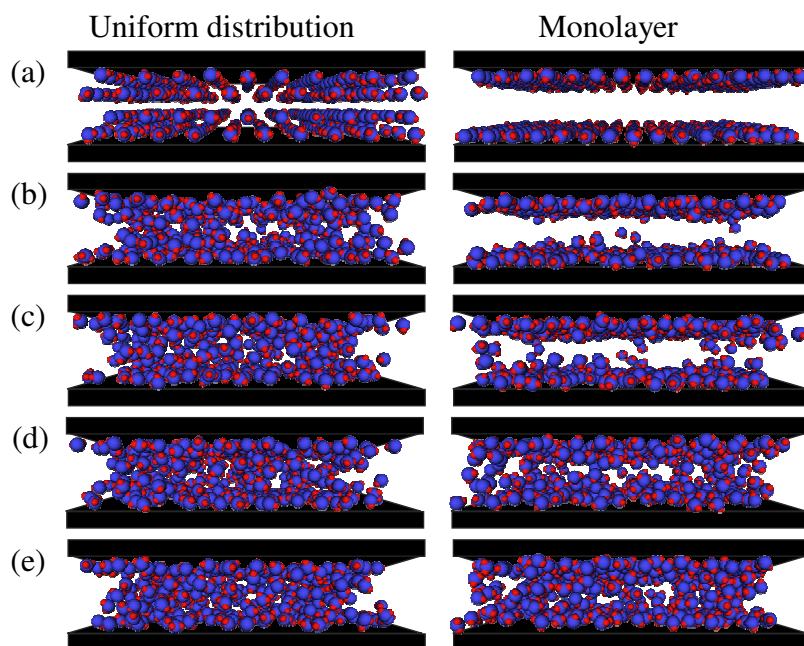


Figure S3. Snapshots showing the uniform distribution structure–cluster and monolayer–cluster transformations at $\phi = 0.2$ in the micropore of $w = 1.1$ nm, as studied by MD simulation. Time scale = 0 (a), 1 (b), 2 (c), 3 (d), and 4 (e) ps.