Supporting Information for

"Dependence of water dynamics on molecular adsorbates near hydrophobic surfaces: A First Principles Molecular Dynamics Study"
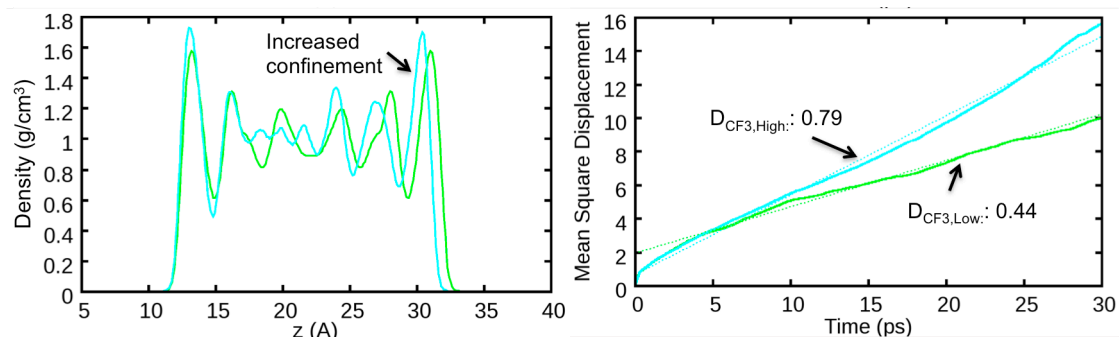
by Donghwa Lee, Eric Schwegler, and Yosuke Kanai

Fig S1. Density (left) and mean square displacement (right) of water molecules at Si surface passivated with CF_3 molecules; Simulation cell with low-confining distance (green) is 0.8 Å larger than that of high-confining distance (cyan). The increased confinement enhances the diffusivity of water from 0.44 to 0.79 ($\times 10^{-5}$ cm^2/s) at CF_3-terminated surface. We note here that water molecules at CF_3-terminated surface with enhanced confining distance shows still slower diffusivity than the water molecules at H-terminated surface with low-confining distance [1.44 ($\times 10^{-5}$ cm^2/s)].
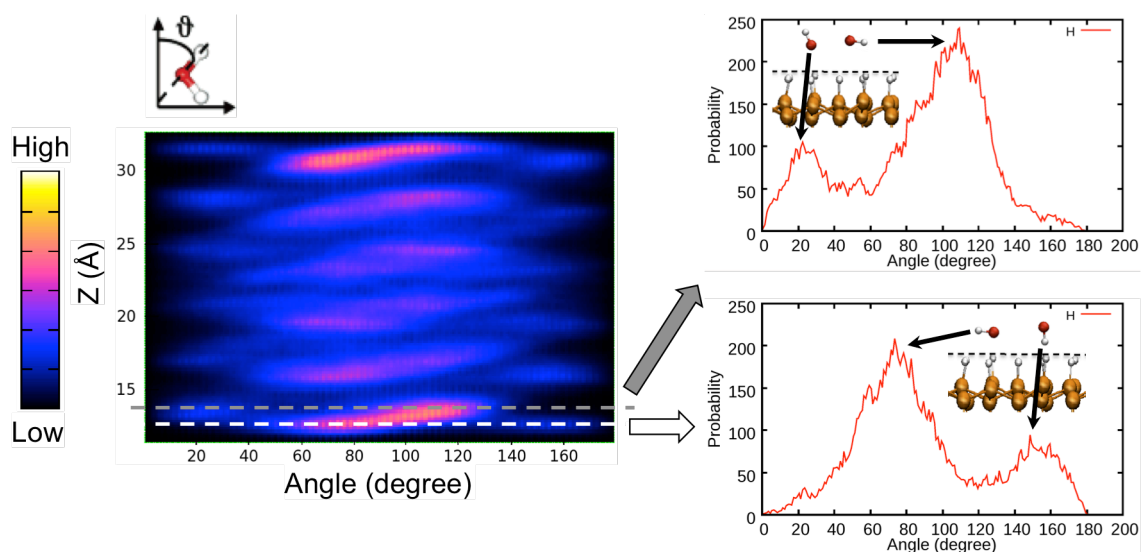
Fig S2. The tilt angle distribution of OH vector for the H-terminated surface (left). The contour map shows the probability of the OH vector angle (shown at the top) as a function of the distance from the surface. Right figures show the distribution of the OH vector at 2.1 Å (lower) and 3.1 Å (upper) away from the surface.
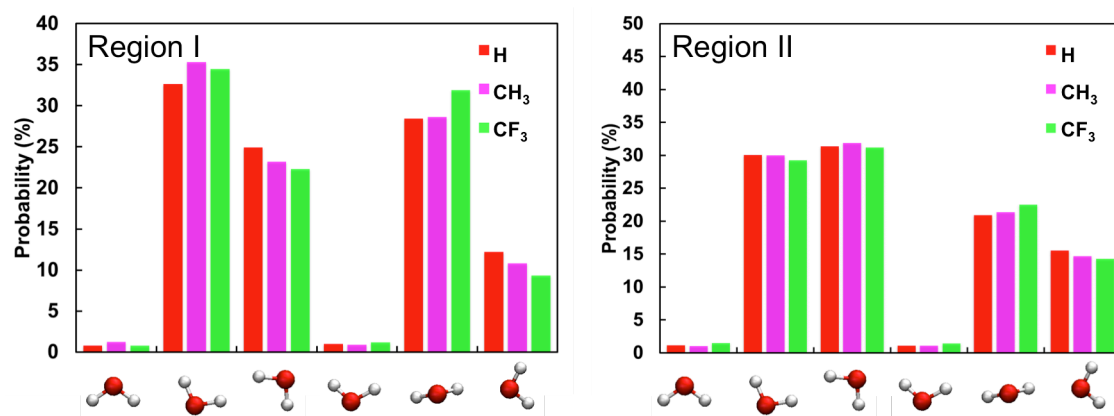
Fig S3. Probability of specific orientation of water molecules in Region I and Regions II (See main text). Molecular orientation of individual waters is classified in six different categories, depending on the orientation of two OH vectors with respect to the surface. The qualitative features are similar for the three non-polar surfaces.
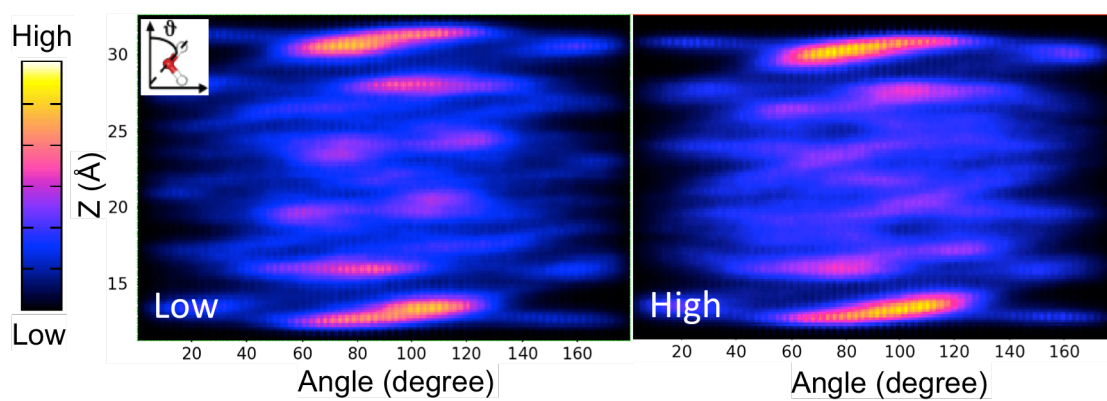
Fig S4. The tilt angle distribution of OH vector at CF_3-terminared surface with two confining distances; Simulation cell with low-confining distance (left) is 0.8 Å larger than that of high-confining distance (right). The distribution of the OH bond orientations remains largely insensitive to the confining distance.