Supporting information for: Friction at ice-I_h / water interfaces is governed by solid-liquid hydrogen-bonding

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Overview

The supporting information contains further details about the model construction, analysis methods, and supplies figures that support the data presented in the main text.

Fitting velocity profiles

In order to calculate solid-liquid friction coefficients, κ from Eq. (5) in the main text, the velocity profiles, $v_x(z)$, obtained from each shearing simulation were fit assuming linear behavior through each of the three regions of the simulation box; the lower liquid, the solid, and the upper liquid. Parabolic functions were designed to capture the negative slip behavior that links the three regions,

$$v(z) = \begin{cases} v_l - m_l z & 0 \leq z < (z_1 - w) \\ v_s - \frac{1}{2}k(z-z_1)^2 & (z_1 - w) \leq z < z_1 \\ v_s & z_1 \leq z < z_2 \\ v_s - \frac{1}{2}k(z-z_2)^2 & z_2 \leq z < (z_2 + w) \\ v_s - \frac{1}{2}kw^2 - m_l(z-(z_2+w)) & (z_2+w) \leq z \end{cases} \tag{1}$$

Here, v_l is the velocity of the liquid at the middle of the liquid domain (the edge of the simulation box), and v_s is the velocity of the solid. The locations z_1 and z_2 are the edges of the ice slab, and w is the width of the interface (distinct from w_{10-90} mentioned in the main text). The parameter m_l is the slope of the velocity profile in the liquid regions of the box which is related to the liquid-state viscosity. Figure S1 shows a representative velocity profile (navy squares) and fit (green line) with the locations of z_1 and z_2 indicated as vertical dotted lines. Once the fits were obtained, the values for $v_x(solid)$ and $v_x(liquid)$ for Eq. (5) were sampled from the fit. The z locations used to sample the fit were determined by structural measures. The z location for $v_x(liquid)$ was taken to be the Gibbs dividing surface of the interface, less the $10-90$ width of the interface. Similarly, the z location for $v_x(solid)$ was taken to be the Gibbs dividing surface plus the $10-90$

width of the interface.

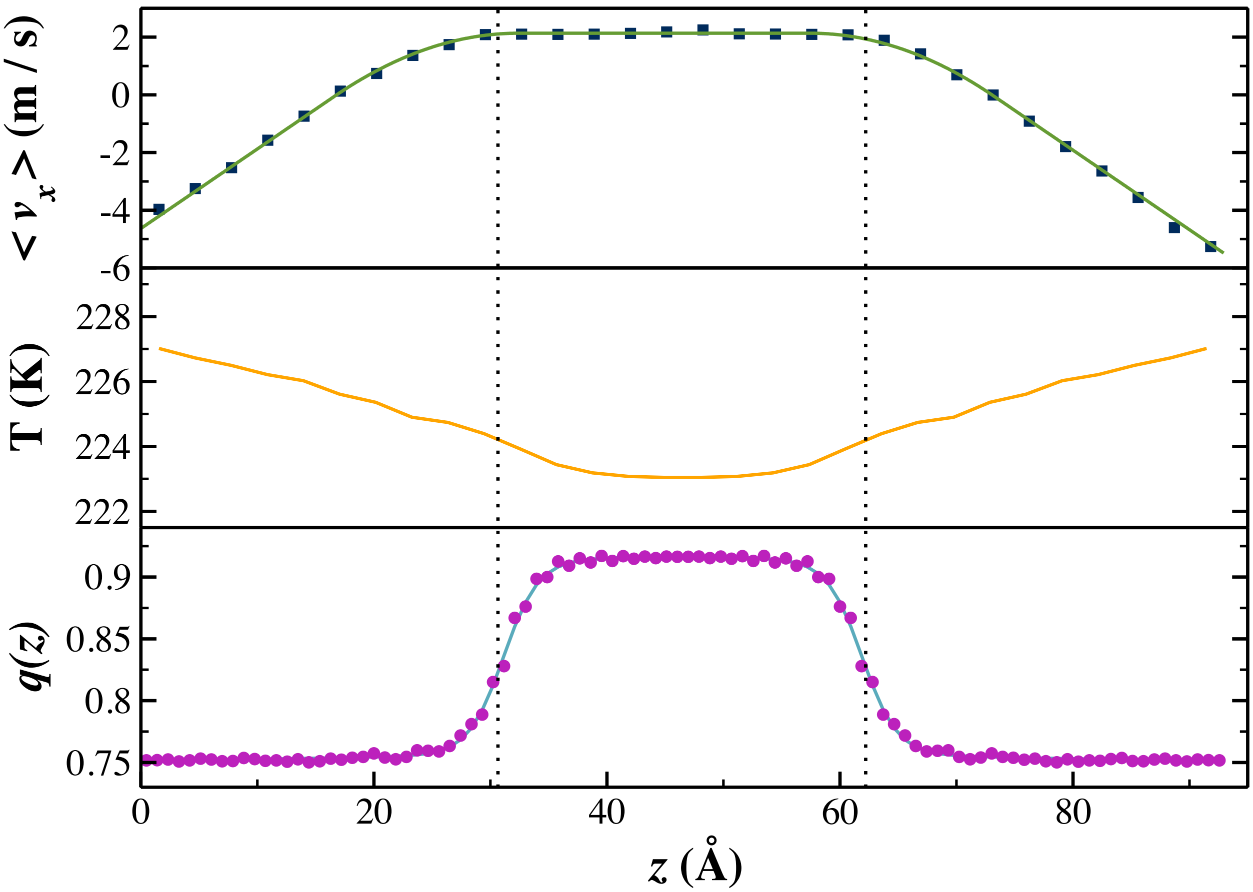

Figure S1: Properties of the pyramidal interface being sheared through water at 7.6 ms^{-1}. Lower panel: the local tetrahedral order parameter, $q(z)$, (circles) and the hyperbolic tangent fit (turquoise line). Middle panel: the imposed thermal gradient required to maintain a fixed interfacial temperature of 225 K. Upper panel: the transverse velocity gradient (squares) that develops in response to an imposed momentum flux, along with the fit (green line). The vertical dotted lines indicate the locations of the Gibbs dividing surfaces of the two interfaces.

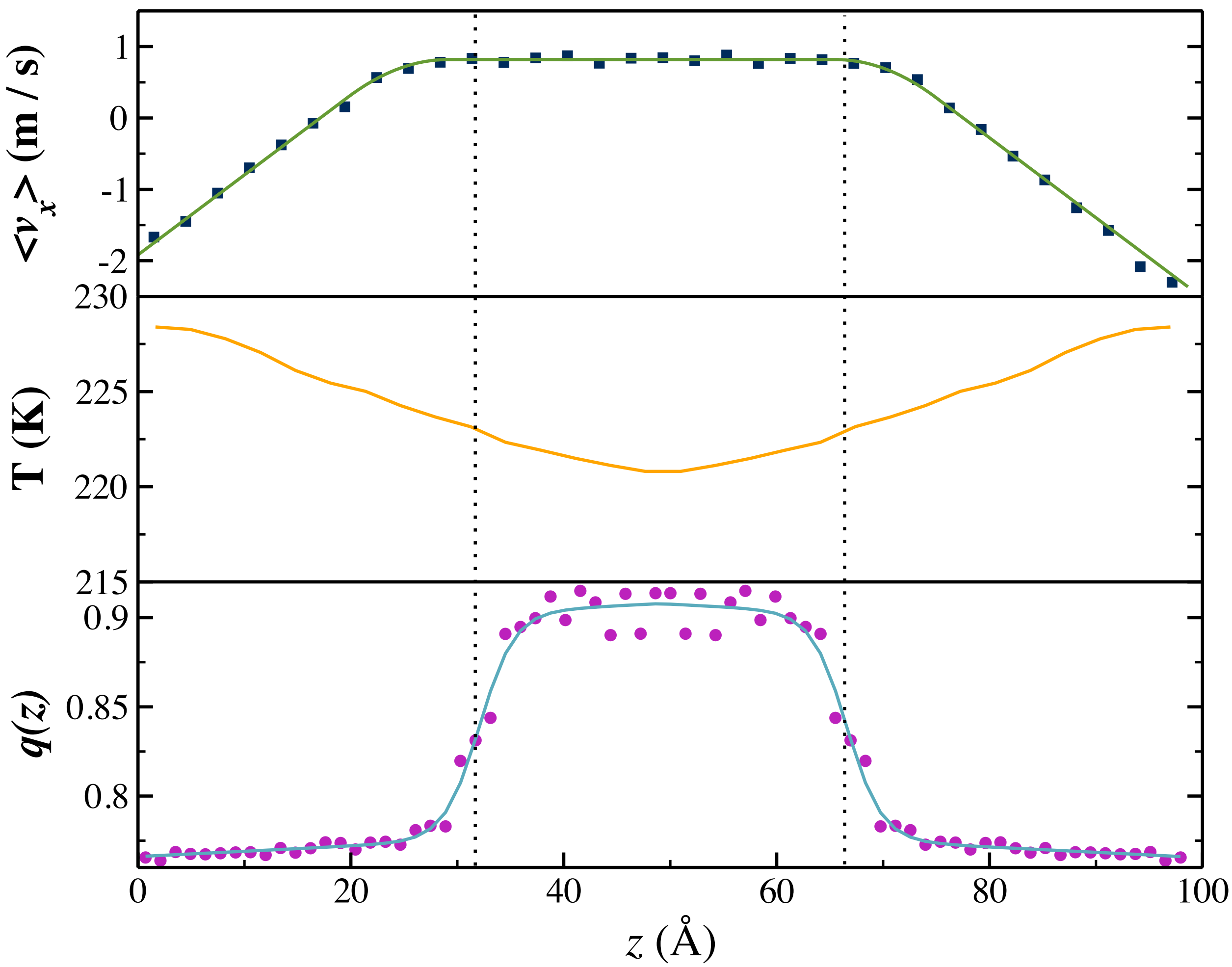

Figure S2: Properties of the basal interface being sheared through water at 3.2 ms^{-1}. Panel descriptions are the same as in Fig. S1.

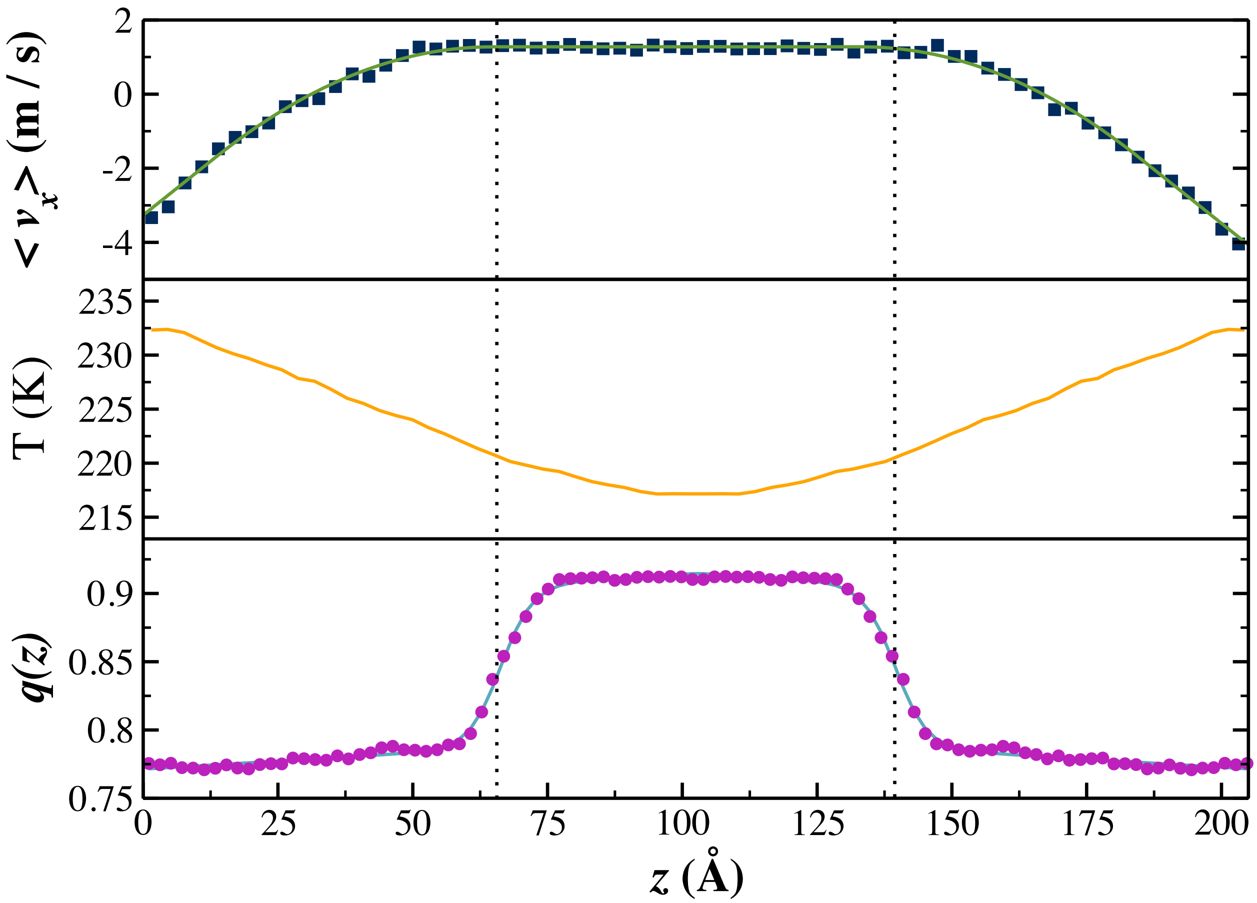

Figure S3: Properties of the prismatic interface being sheared through water at 6.0 ms^{-1}. Panel descriptions are the same as in Fig. S1.

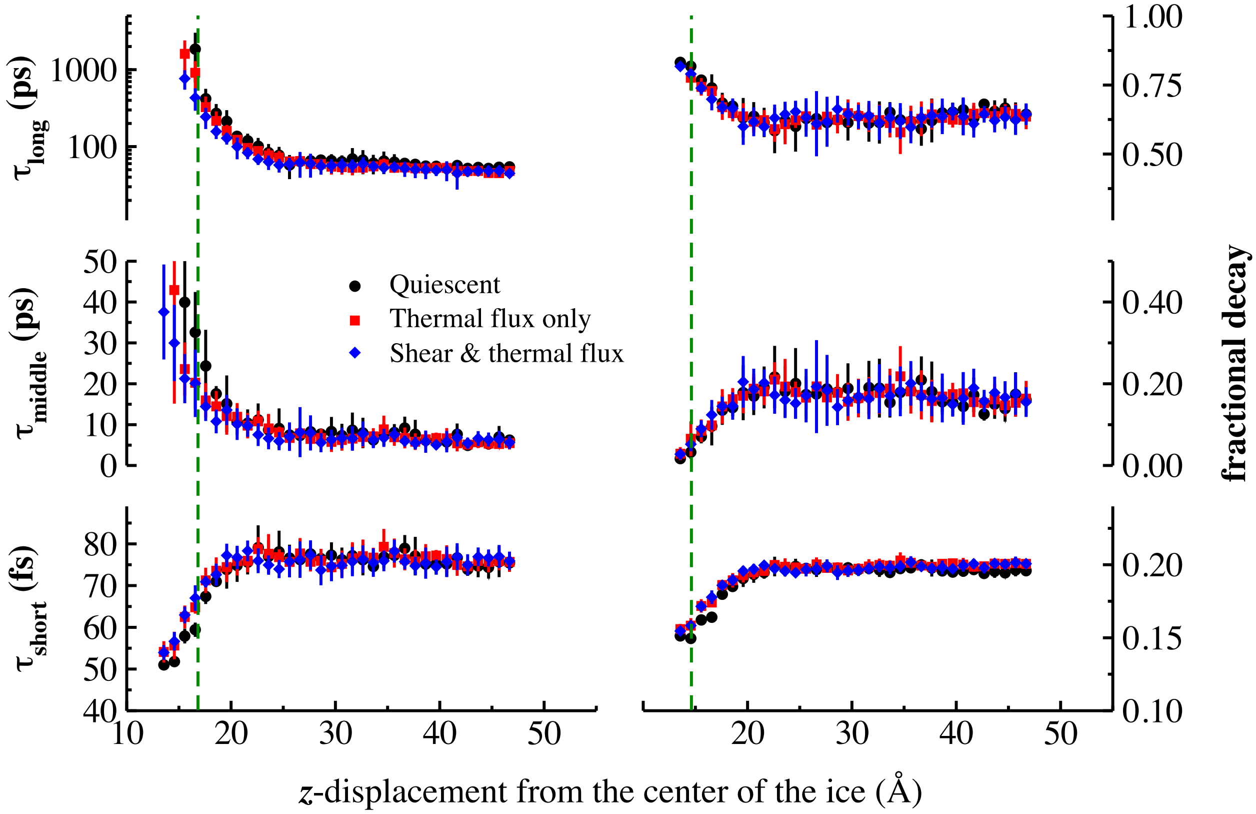

Figure S4: Decay times (left) for $C_2(z,t)$ at the pyramidal interface, and their fractional contributions to the overall decay (right) fit using Eq. (8). The local decay constants are plotted as a function of distance from the center of the ice slab. The vertical dashed line indicates the Gibbs dividing surface determined using the local tetrahedral order parameter. Results are shown for a quiescent system with no applied kinetic or momentum flux (black), an interface with with an imposed kinetic energy flux (red), and a sheared simulation (blue) with both kinetic and momentum fluxes.

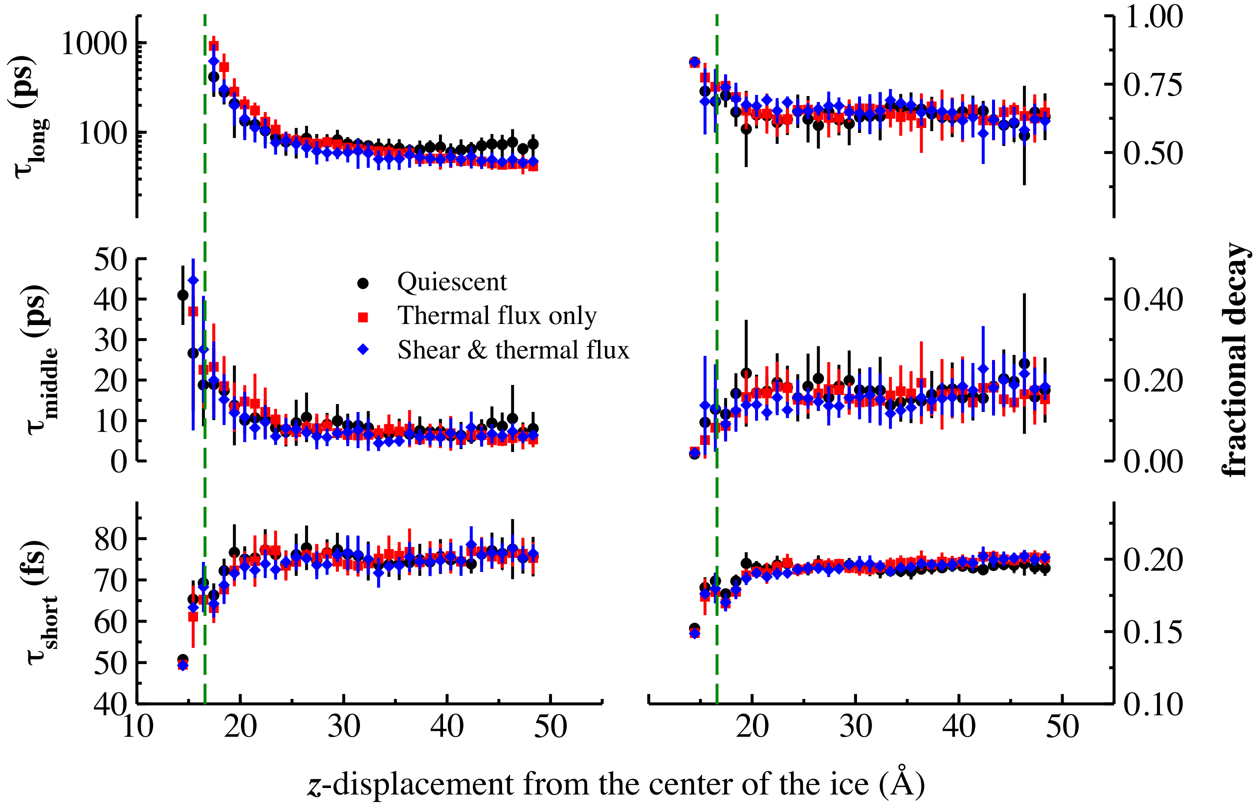

Figure S5: $C_2(z,t)$ time constants for the basal interface. Panel descriptions are the same as in Fig. S4.

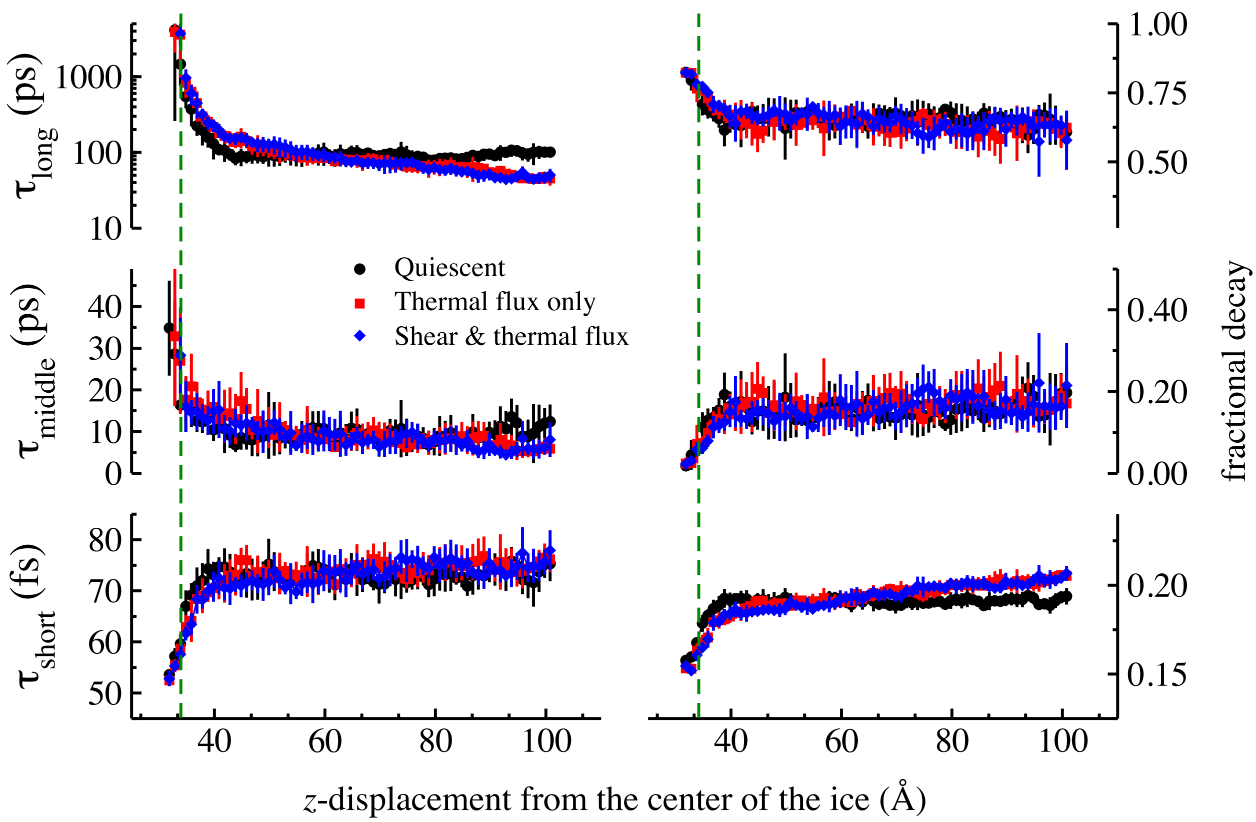

Figure S6: $C_2(z,t)$ time constants for the prismatic interface. Panel descriptions are the same as in Fig. S4.

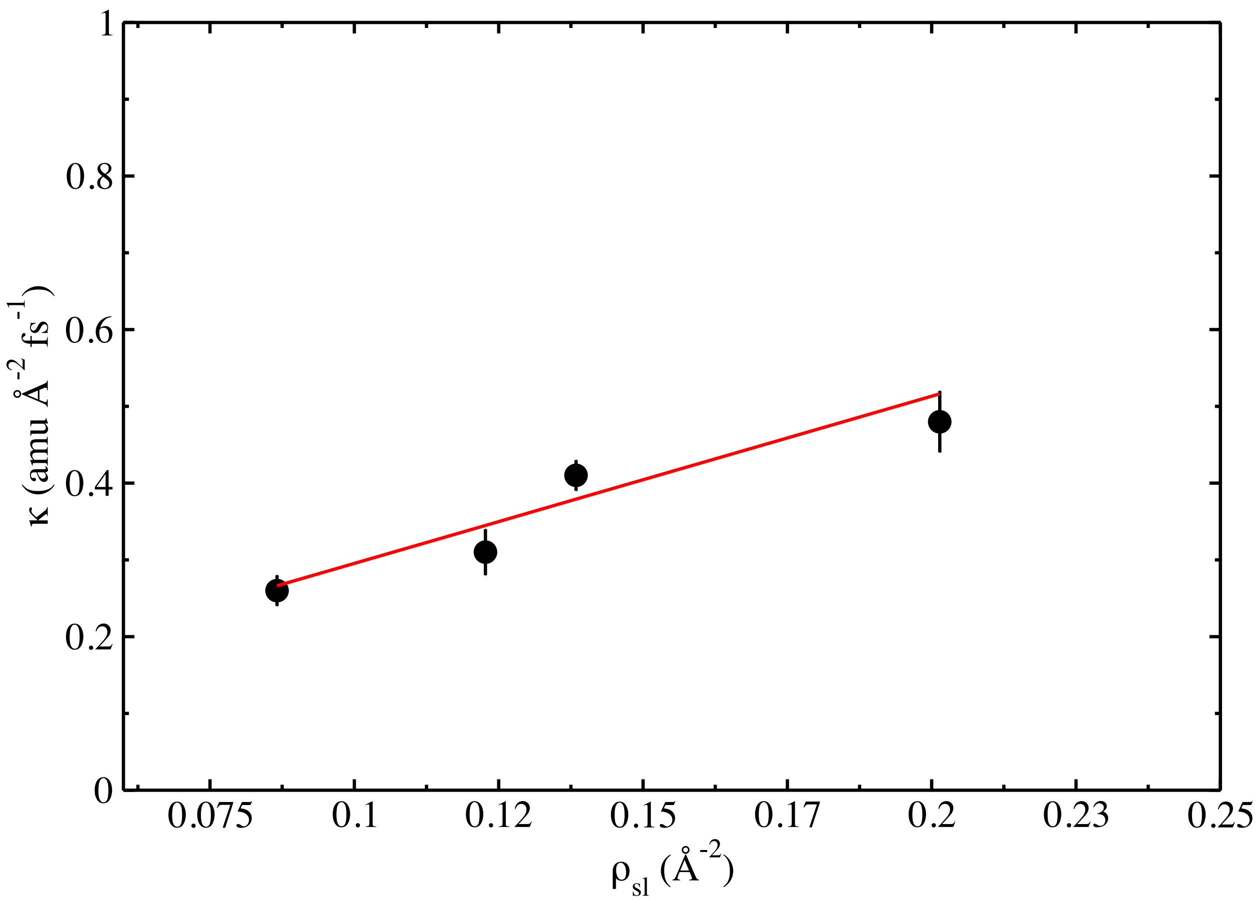

Figure S7: Solid-liquid friction coefficients by the surface density of hydrogen bonds. Linear regression gives a slope of 2.1772 (amu fs^{-1}) and a y-intercept of 0.0777 (amu $Å^{-2}$ fs^{-1}).