

## **Supplemental Material**

**for**

### **How Clay Delamination Supports Aseismic Slip**

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# S1. Molecular volume of bulk water

The molecular volume of bulk water ( $V_f$ ) is derived through the equilibrium simulation. Fig. S1 shows  $V_f$  as a function of water pressure ( $P_f$ ).  $V_f(P_f)$  can be fitted with a third-order polynomial equation. Fitting parameters are shown in Table S1.

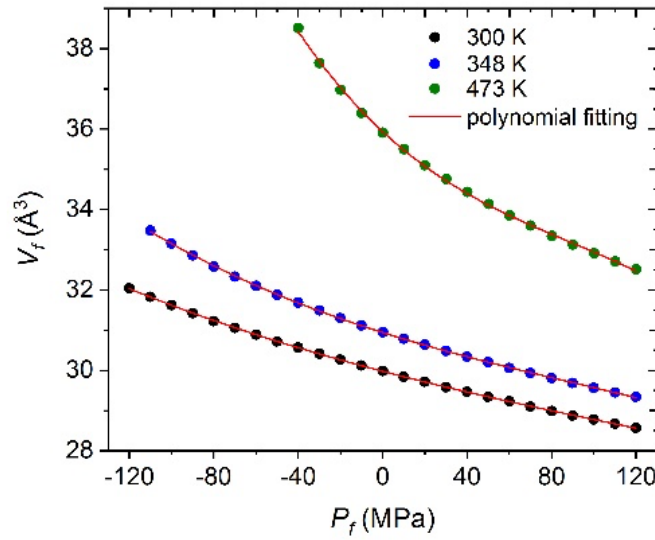


FIGURE S1. The molecular volume of bulk water ( $V_f$ ) as a function of water pressure ( $P_f$ ).

TABLE S1. Polynomial fitting parameters. The fitting equation is  $V_f = a_1P_f^3 + a_2P_f^2 + a_3P_f + b$ .

Temperature (K)	$a_1$	$a_2$	$a_3$	$b$
300	$-5.392 \times 10^{-8}$	$2.212 \times 10^{-5}$	$-1.368 \times 10^{-2}$	$2.998 \times 10^1$
348	$-1.424 \times 10^{-7}$	$4.196 \times 10^{-5}$	$-1.648 \times 10^{-2}$	$3.094 \times 10^1$
473	$-1.113 \times 10^{-6}$	$2.975 \times 10^{-4}$	$-4.858 \times 10^{-2}$	$3.593 \times 10^1$

## S2. Derivation of chemical potential of a water molecule with thermodynamics integrations

The chemical potential ( $\mu$ ) of water either confined in the clay interlayer or in the bulk phase consists of two contributions:

$$\mu = \mu^I + \mu^\times \quad (\text{S1})$$

where  $\mu^I$  is the chemical potential of the ideal gas state, and  $\mu^\times$  is the excess chemical potential.  $\mu^I$  depends on density ( $\rho$ ) of water and expressed as  $\mu^I = k_B T \ln \rho + C$ , where  $C$  is a constant related to the internal partition function of an isolated molecule (Ben-Amotz 2016). The excess chemical potential  $\mu^\times$ , can be derived with thermodynamics integrations.  $\delta N$  water molecules are arbitrarily selected from the equilibrium configuration.  $\lambda = 0$  is the state with intact Lennard-Jones (LJ) and Coulombic interactions. In the  $\lambda = 1$  state, those interactions are eliminated for selected molecules. Coulomb and LJ interactions are eliminated sequentially through continually increasing  $\lambda$  from 0 to 1. In each state, a stochastic dynamics simulation in  $\text{NP}_\sigma\text{T}$  ensemble is run for 0.3 ns. The last 0.1 ns data are for computing instantaneous enthalpy derivative  $\partial H(\lambda)/\partial \lambda$ .  $\mu^\times$  is derived through the integration:

$$\mu^\times \approx -\frac{1}{\delta N} \int_0^1 \left\langle \frac{\partial H(\lambda)}{\partial \lambda} \right\rangle_\lambda d\lambda \quad (\text{S2})$$

$\mu^\times$  are estimated with the Bennett acceptance ratio method (Pohorille et al. 2010).

### S3. Velocity of the pulled group as a function of shear stress

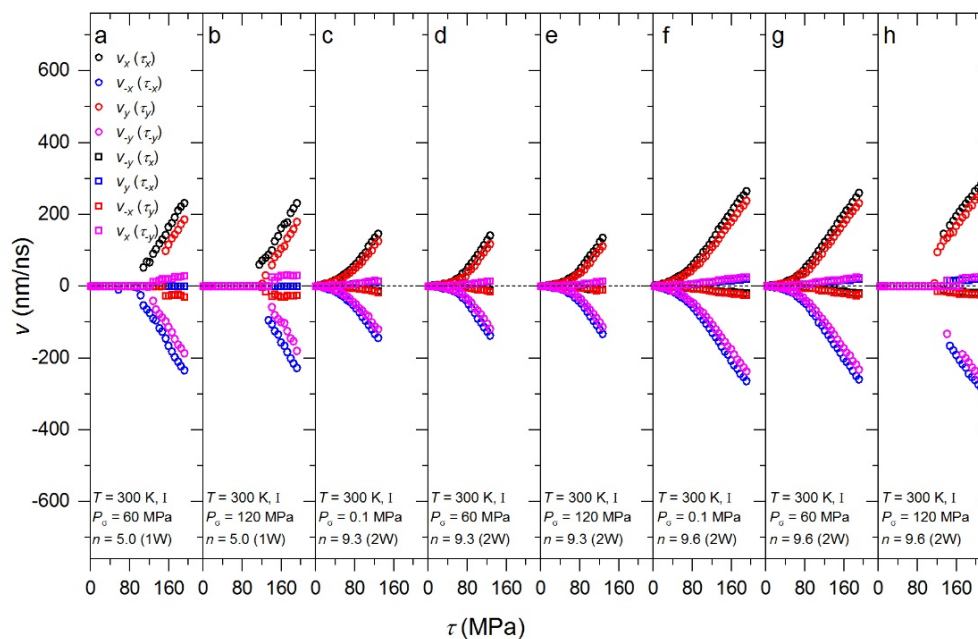


FIGURE S2. Velocity component of the pulled group as a function of the shear stress ( $\tau$ ) at 300 K. Subscripts ( $x$ ,  $-x$ ,  $y$ , and  $-y$ ) denote shear direction or direction of velocity component. “I” denotes that separate thermostat was used.

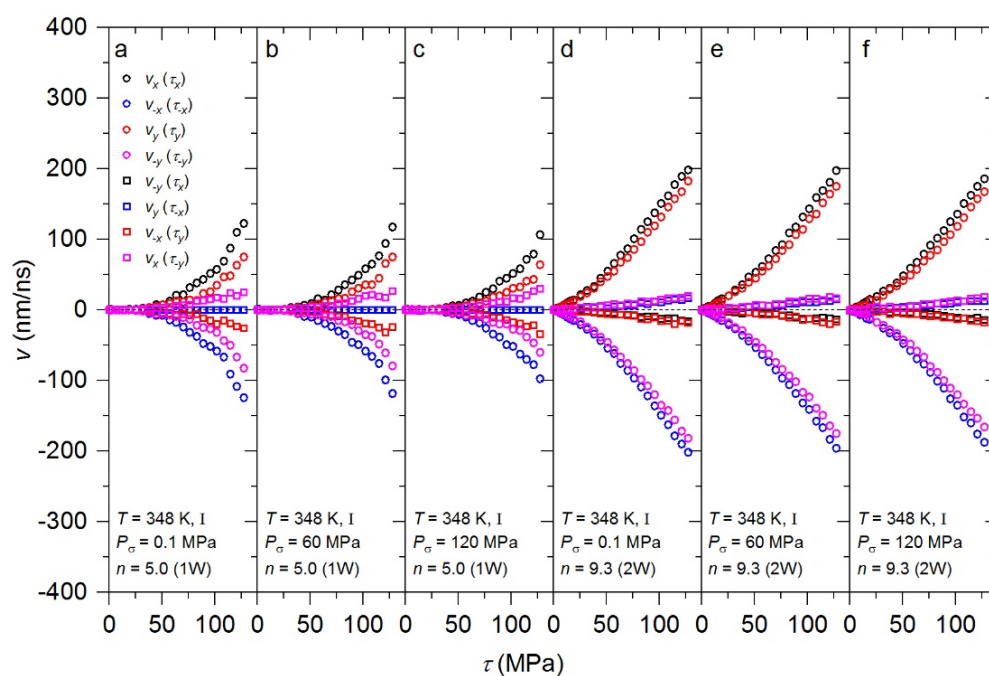


FIGURE S3. Velocity component of the pulled group as a function of the shear stress ( $\tau$ ) at 348 K. Subscripts ( $x$ ,  $-x$ ,  $y$ , and  $-y$ ) denote shear direction or direction of velocity component. “I” denotes that separate thermostat was used.



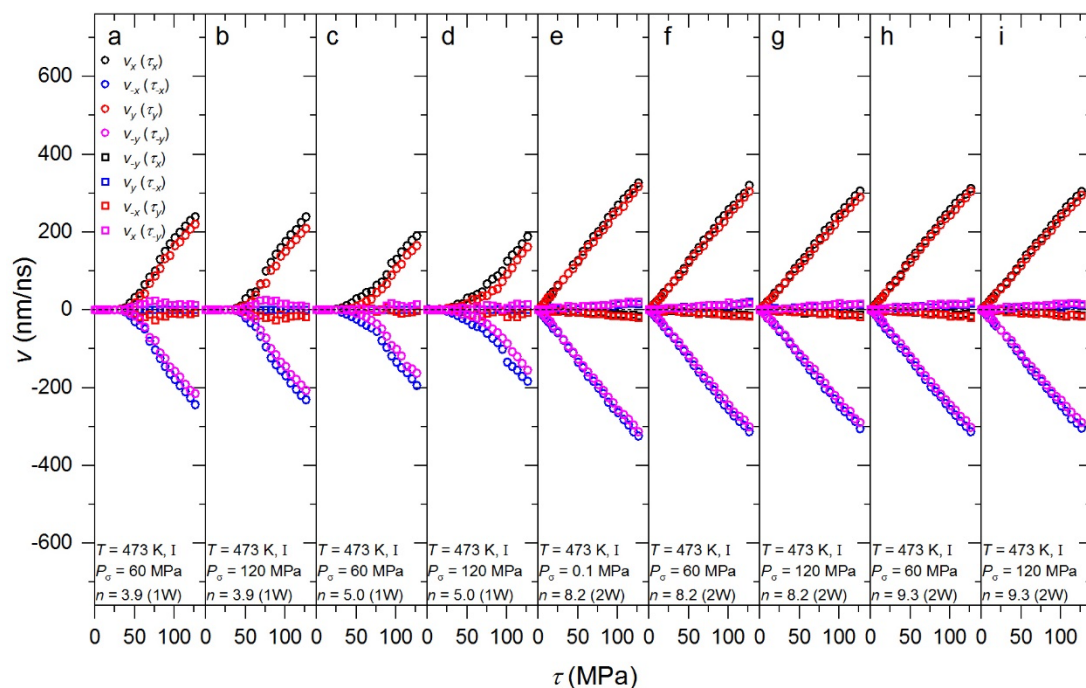


FIGURE S4. Velocity component of the pulled group as a function of the shear stress ( $\tau$ ) at 473 K. Subscripts ( $x$ ,  $-x$ ,  $y$ , and  $-y$ ) denote shear direction or direction of velocity component. “I” denotes that separate thermostat was used.

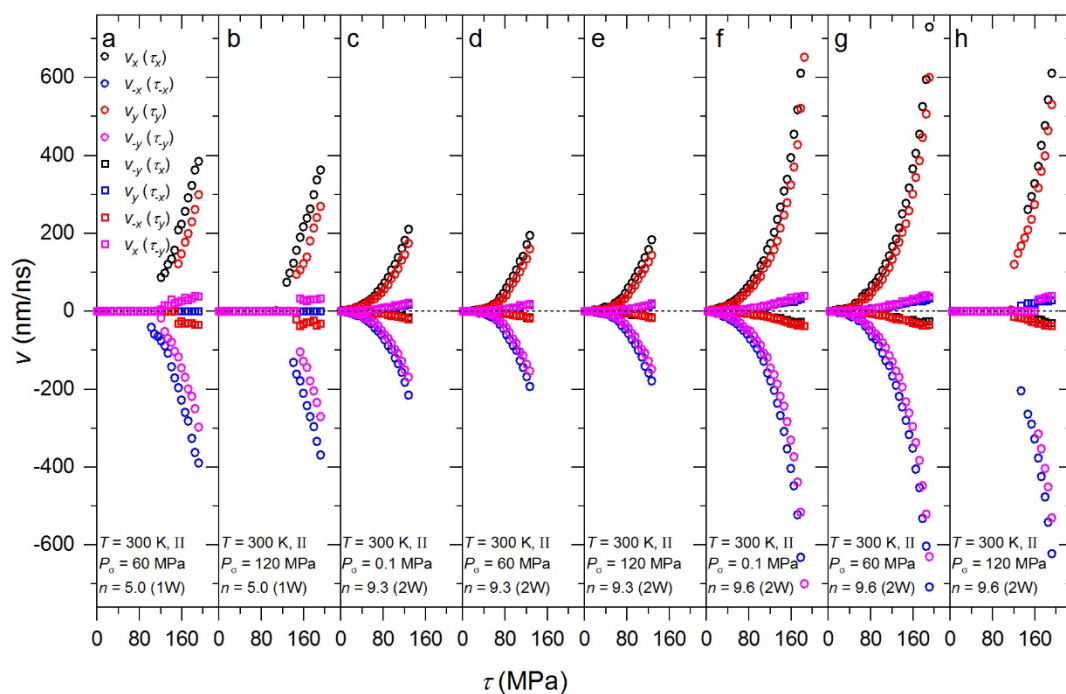


FIGURE S5. Velocity component of the pulled group as a function of the shear stress ( $\tau$ ) at 300 K. Subscripts ( $x$ ,  $-x$ ,  $y$ , and  $-y$ ) denote shear direction or direction of velocity component. “II” denotes that partial thermostat was used.

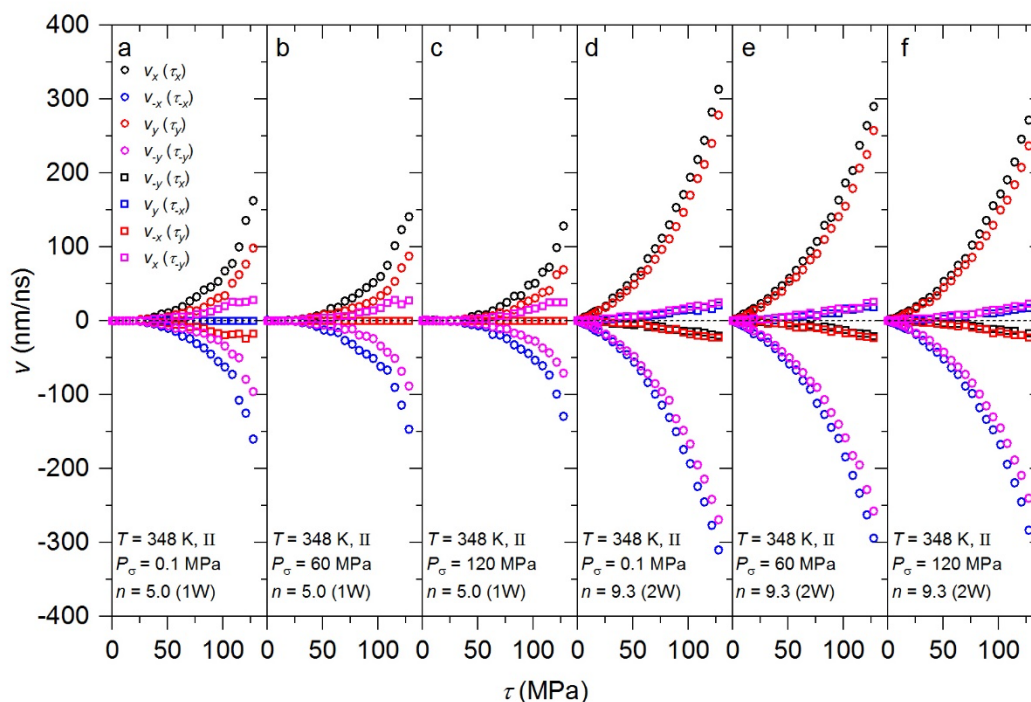


FIGURE S6. Velocity component of the pulled group as a function of the shear stress ( $\tau$ ) at 348 K. Subscripts ( $x$ ,  $-x$ ,  $y$ , and  $-y$ ) denote shear direction or direction of velocity component. “II” denotes that partial thermostat was used.

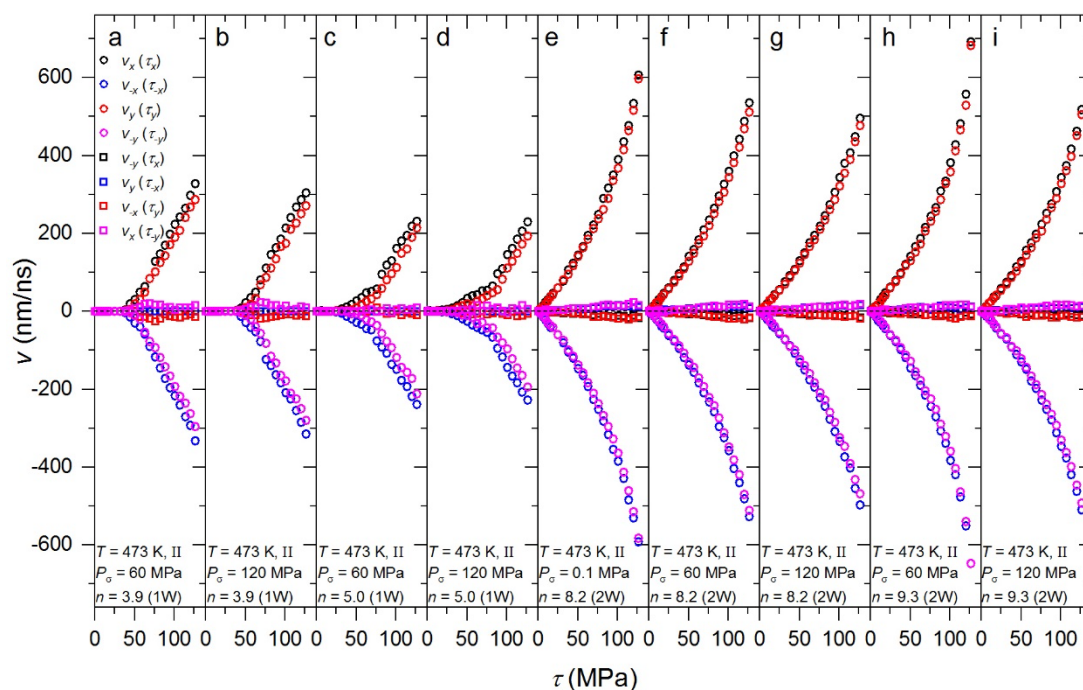


FIGURE S7. Velocity component of the pulled group as a function of the shear stress ( $\tau$ ) at 473 K. Subscripts ( $x$ ,  $-x$ ,  $y$ , and  $-y$ ) denote shear direction or direction of velocity component. “II” denotes that partial thermostat was used.

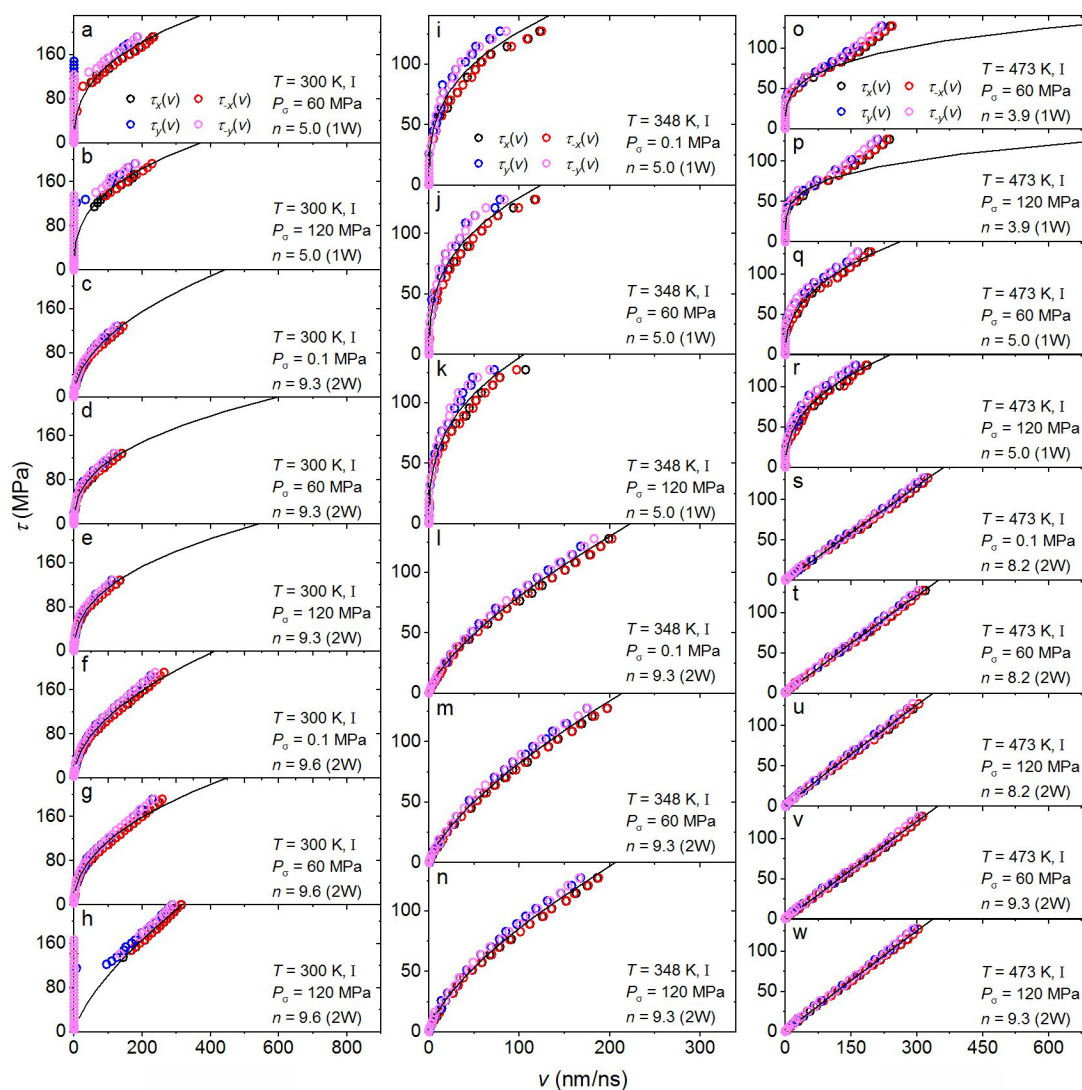


FIGURE S8. Shear stress ( $\tau$ ) as a function of velocity magnitude ( $v$ ) of the pulled group at 300 K (left), 348 K (middle), and 473 K (right). Subscripts ( $x$ ,  $-x$ ,  $y$ , and  $-y$ ) denote shear directions. Fittings with Eq. (12) in the main text are shown. “I” denotes that separate thermostat was used.

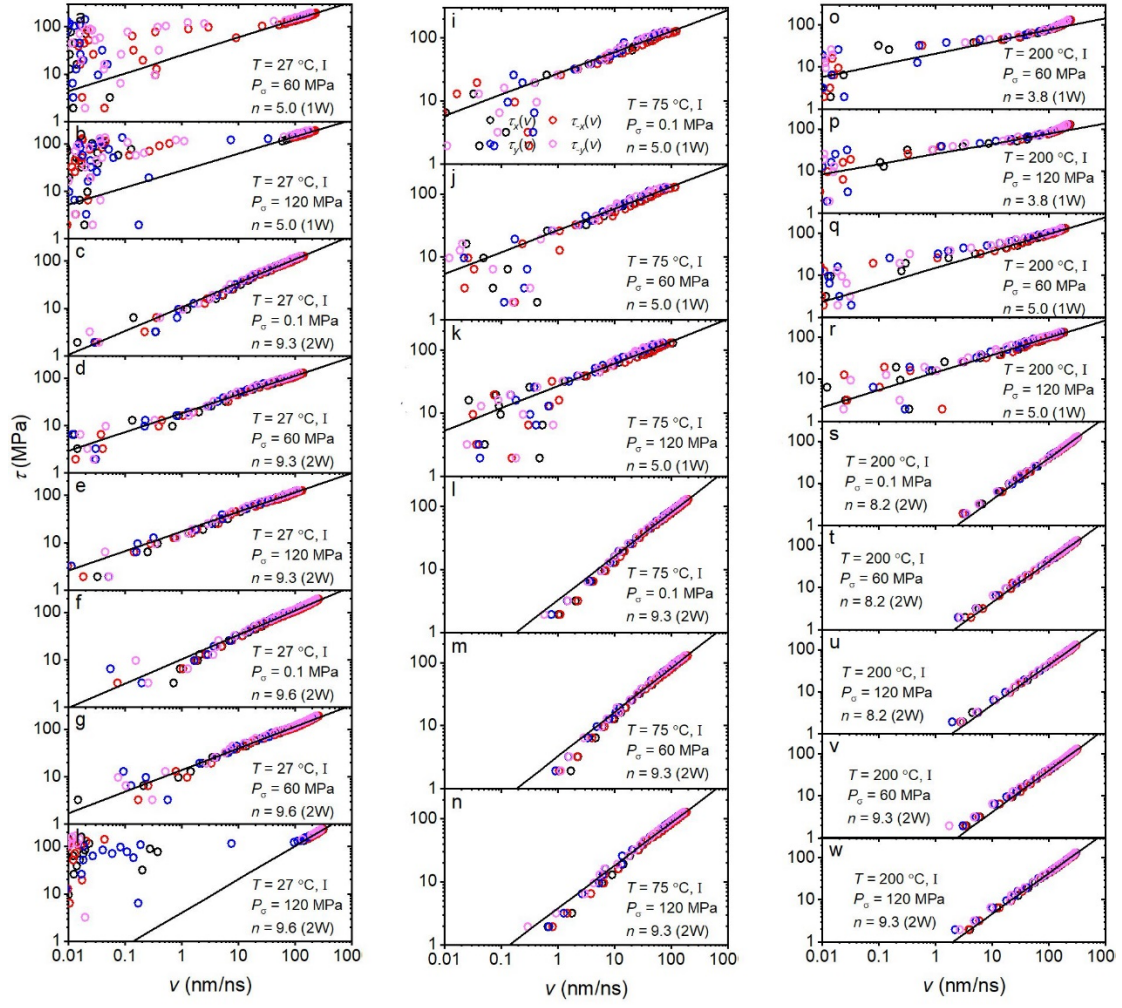


FIGURE S9. The same as Figure S8 except that log-log plots are used.



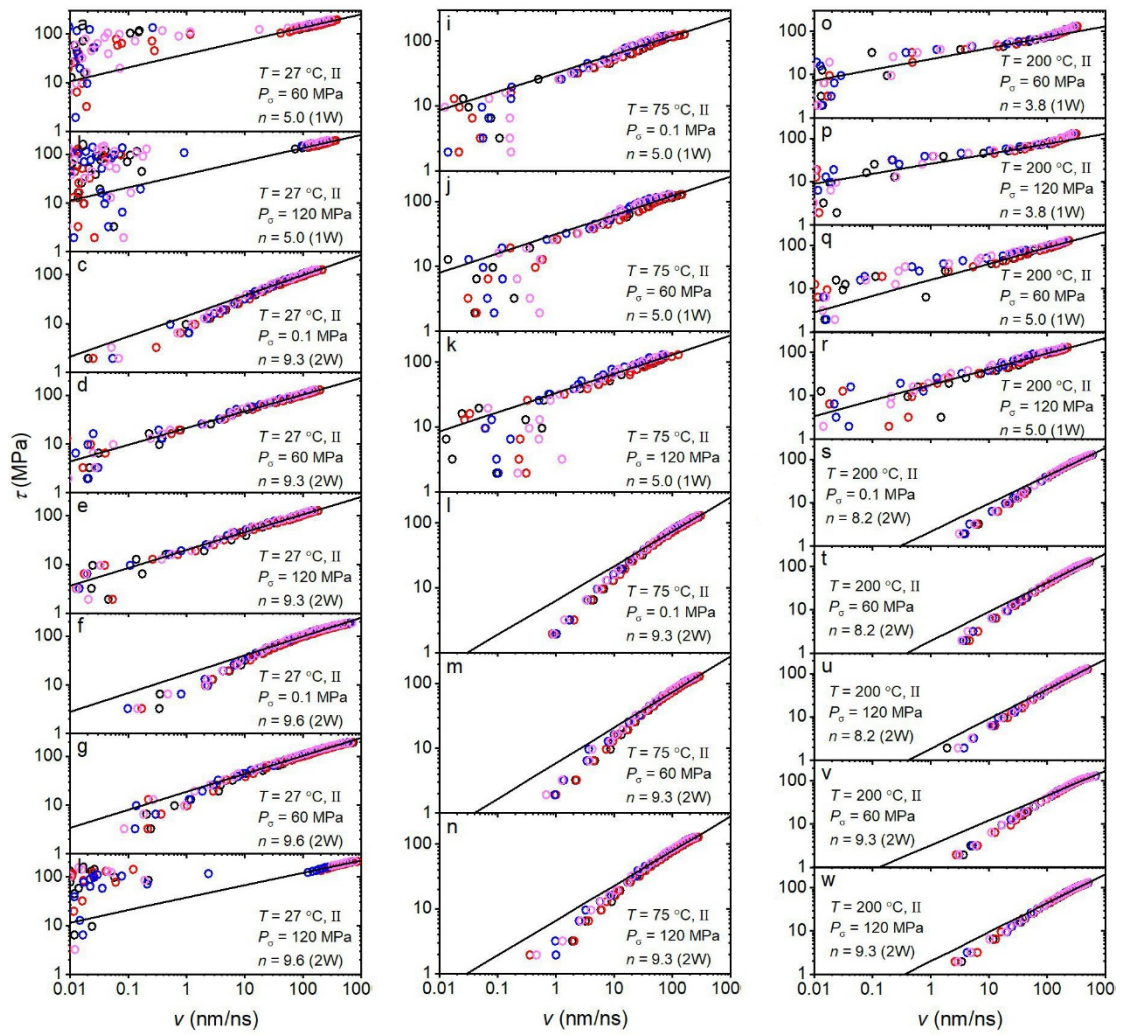


FIGURE S10. The same as Figure S9 except that they are results with partial thermostat.

# S4. The effective viscosity of interlayer water as a function of shear rate

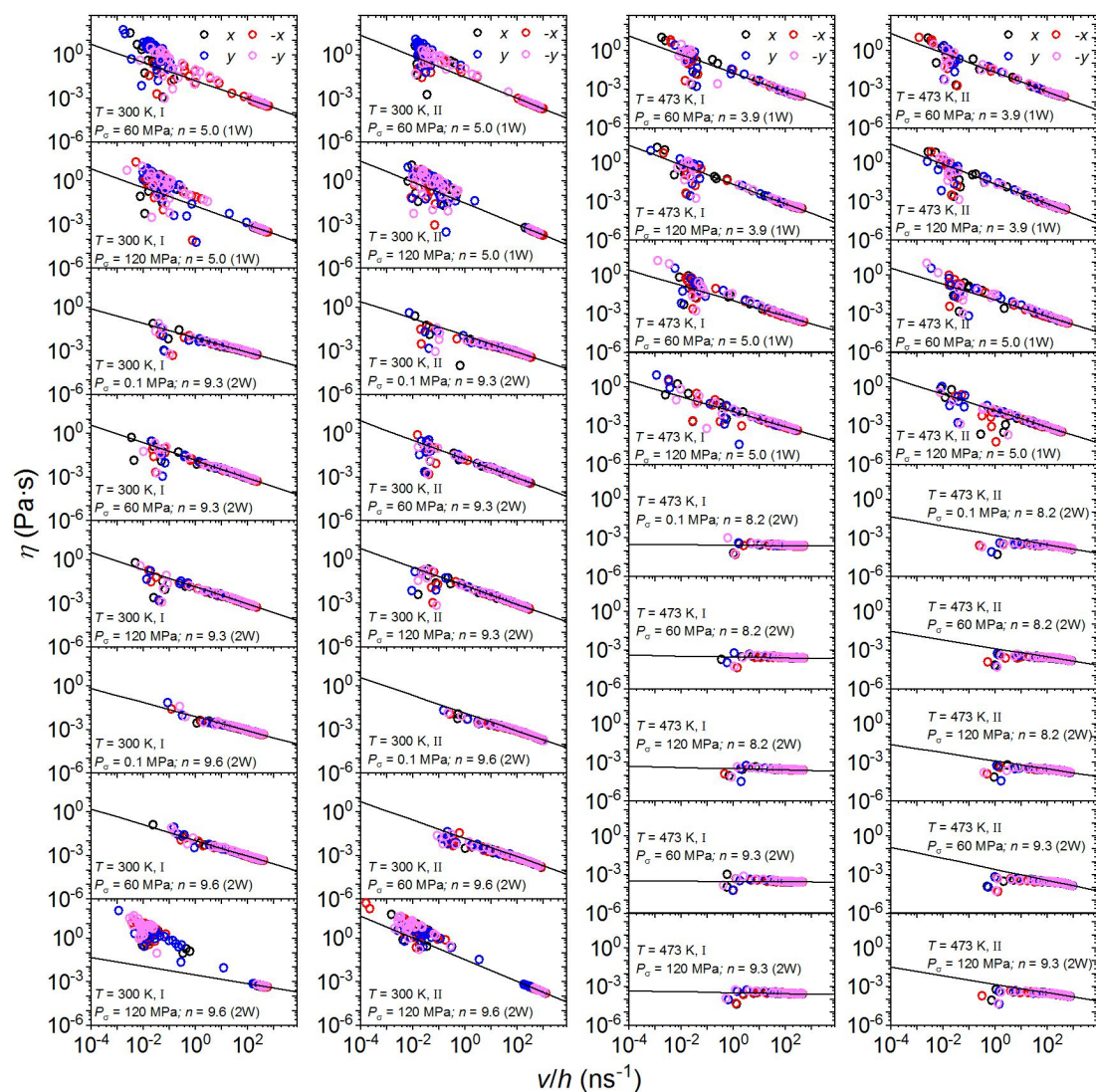


FIGURE S11. The effective viscosity ( $\eta$ ) as a function of shear rate ( $v/h$ ) at 300 and 473 K. “I” and “II” denote results with separate and partial thermostats, respectively. Results with different shear directions ( $x$ ,  $-x$ ,  $y$ , and  $-y$ ) are designated by different colors.

## References

- Ben-Amotz, D. (2016) Interfacial solvation thermodynamics, *Journal of Physics-Condensed Matter*. 28(41), 414013.
- Pohorille, A., Jarzynski, C., and Chipot, C. (2010) Good practices in free-energy calculations, *The Journal of Physical Chemistry B*. 114(32), 10235-10253.