water

MDPI

Supplementary Materials

Structure and Dynamics of Interfacial Water on Muscovite Surface under Different Temperature Conditions (298 K to 673 K): Molecular Dynamics Investigation

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Table S1. Distance between two muscovite surfaces (nm); note that the number of H_2O molecules at 0.1 MPa/523 K and 0.1 MPa/573 K is 1000 while that at other conditions is 1400.

Pressure (MPa)	Temperature (K)								
	298	**323**	**373**	**423**	**473**	**523**	**573**	**623**	**673**
0.1	4.9	5.0	5.1	5.4	5.8	4.5	5.1	-	-
10.0	4.9	4.9	5.1	5.4	5.7	6.2	7.1	10.1	-
50.0	4.8	4.9	5.0	5.2	5.5	5.9	6.4	7.2	8.7

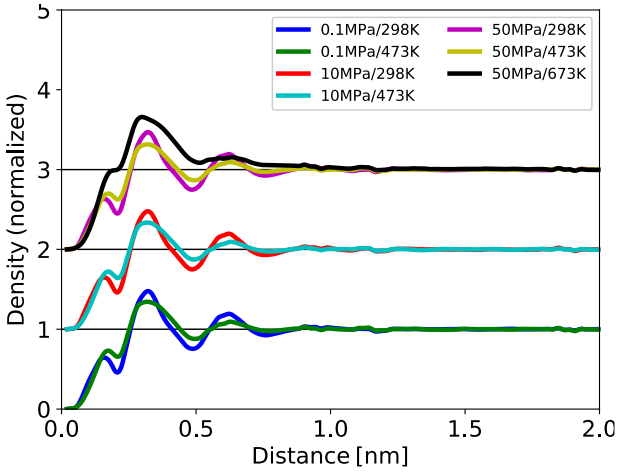


Figure S1. Normalized density profiles of H_2O. Plots have been shifted for clarity.

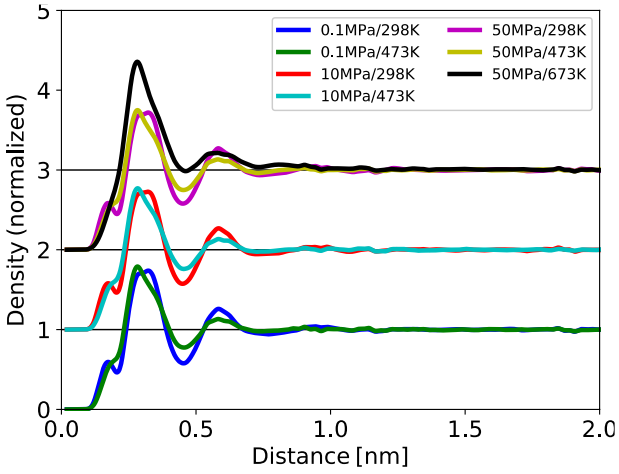


Figure S2. Normalized density profiles of oxygen of H_2O. Plots have been shifted for clarity.

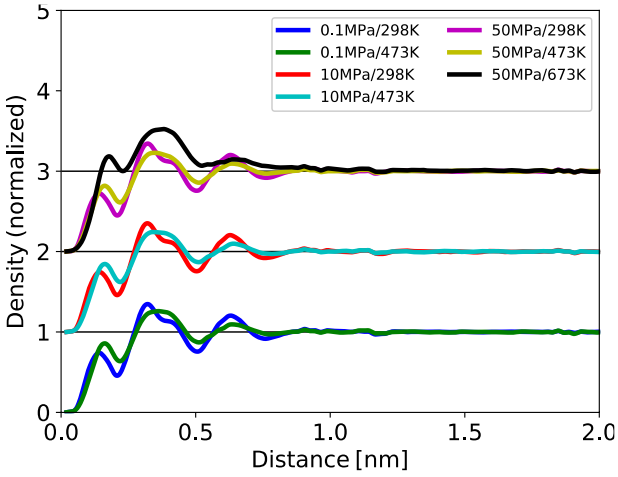


Figure S3. Normalized density profiles of hydrogen of H_2O. Plots have been shifted for clarity.

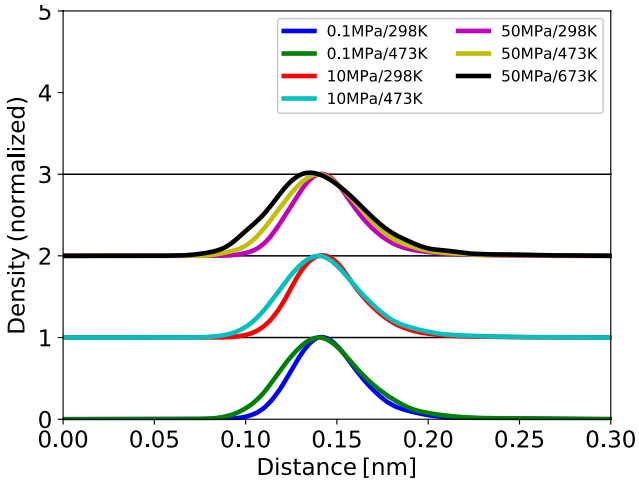
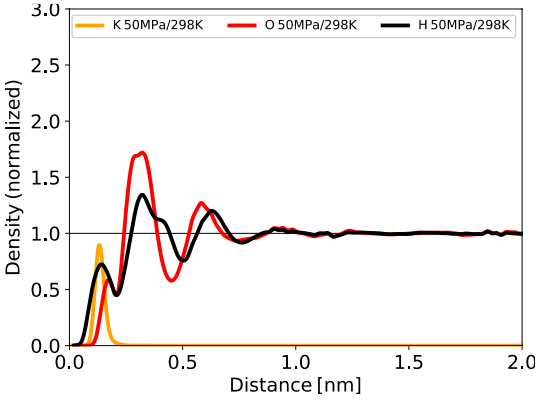
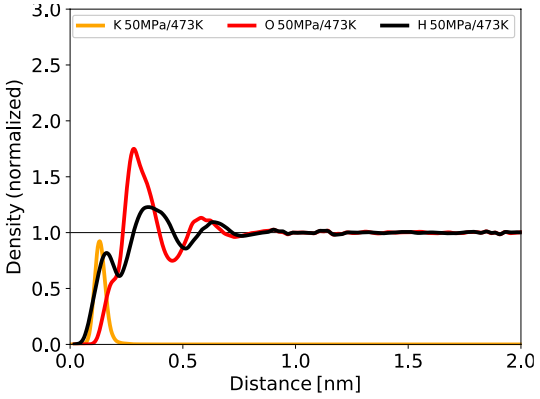


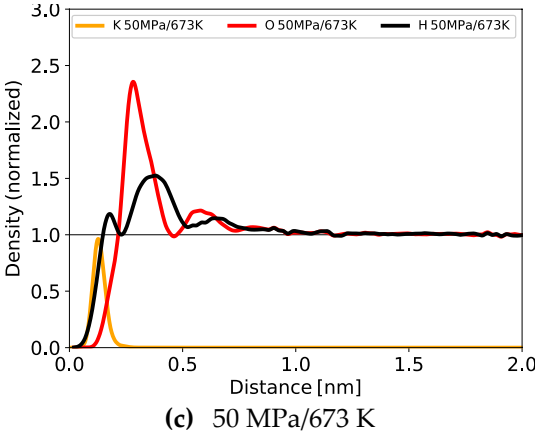
Figure S4. Normalized density profiles of K^+ on the muscovite surface. Plots have been shifted for clarity.



(a) 50 MPa/298 K

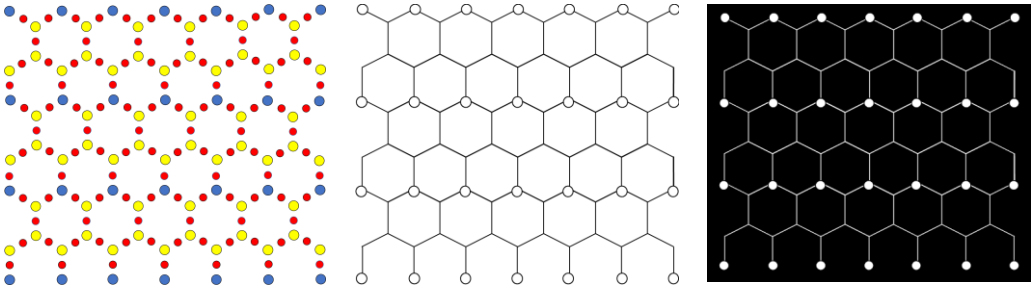


(b) 50 MPa/473 K



(c) 50 MPa/673 K

Figure S5. Normalized density profiles of K^+, O (H_2O), and H (H_2O). Plots have been shifted for clarity.



(**a**) (**b**) (**c**)

Figure S6. Schematic images of the lattice of (0 0 1) surface of muscovite; Al is represented by the blue circles in (**a**) and the white circles in (**b**) and (**c**).

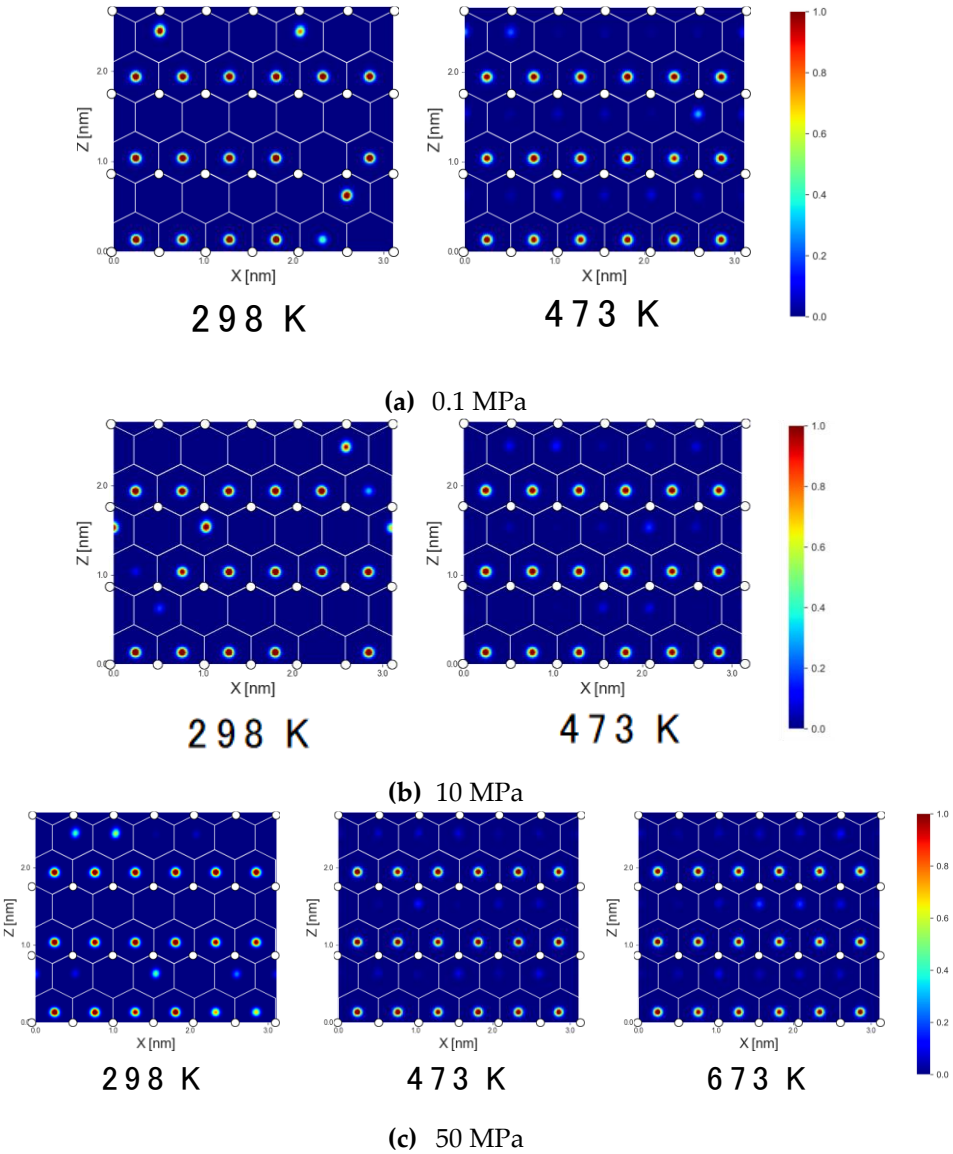


Figure S7. 2D normalized density maps of K^+ on the muscovite surface; the lattice on the map is from Figure S6.

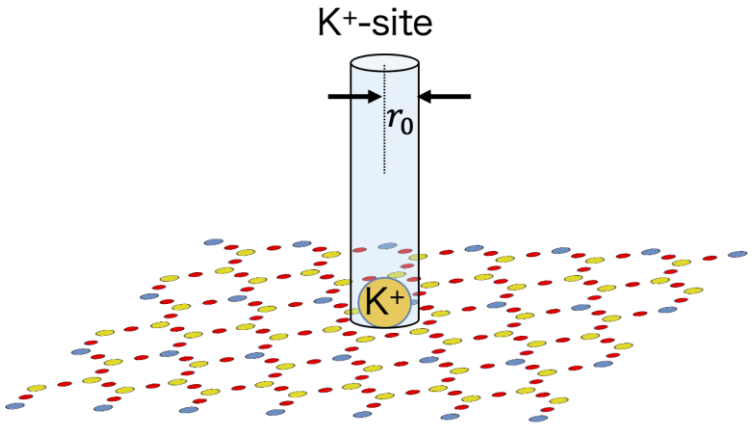


Figure S8. Schematic image of one K^+-site for calculating profiles of density and the orientation angle: r_0 was set to be 0.138 nm, which is the ionic radius of K^+.

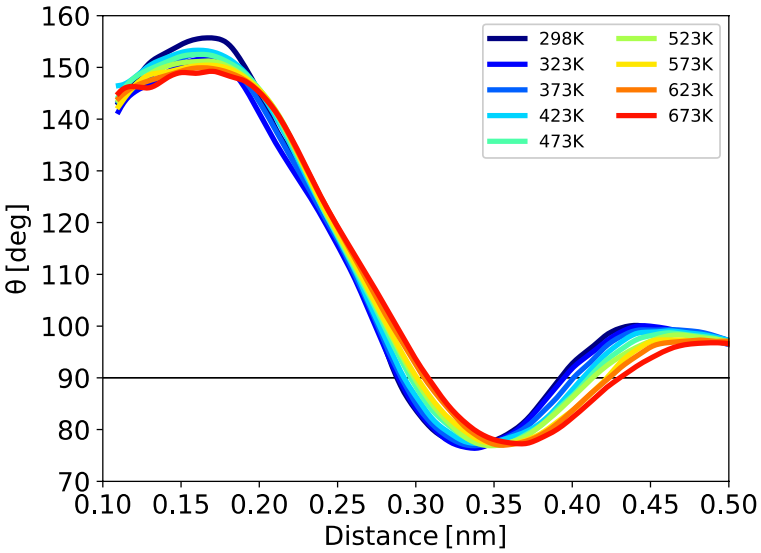


Figure S9. Enlarged view of Figure 8c; 1D profiles of the orientation angle θ from the muscovite surface at 50 MPa.

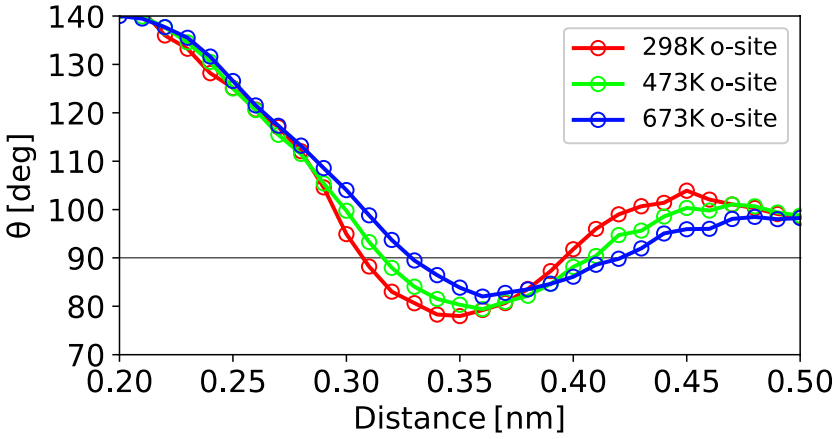


Figure S10. Enlarged view of the part of Figure 10; 1D Profiles of the orientation angle θ on o-site in the second layer (0.2 nm < d < 0.5 nm).

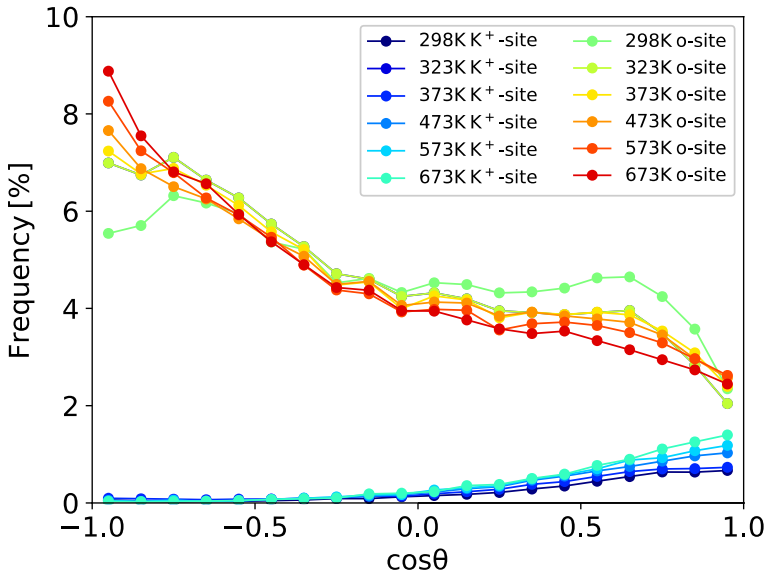


Figure S11. Distributions of cosθ on K^+-site and o-site at the second layer at 50 MPa.

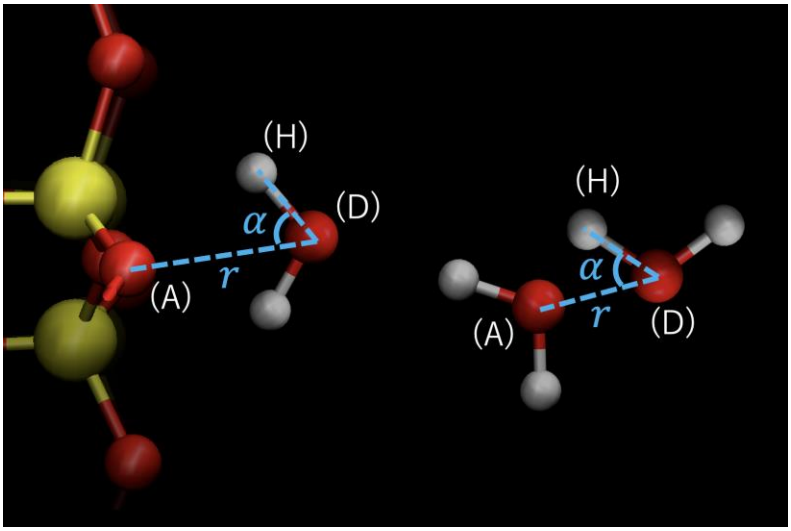
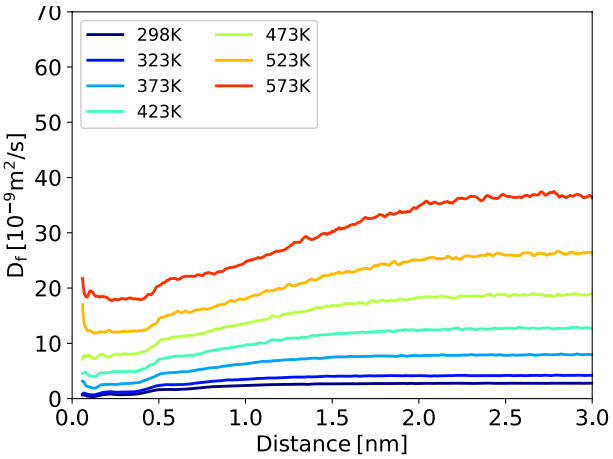
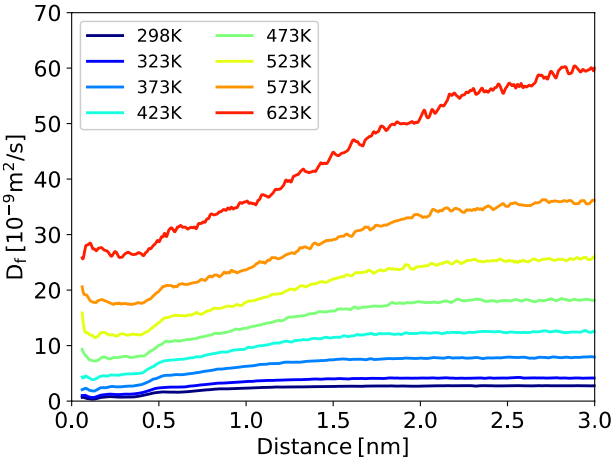


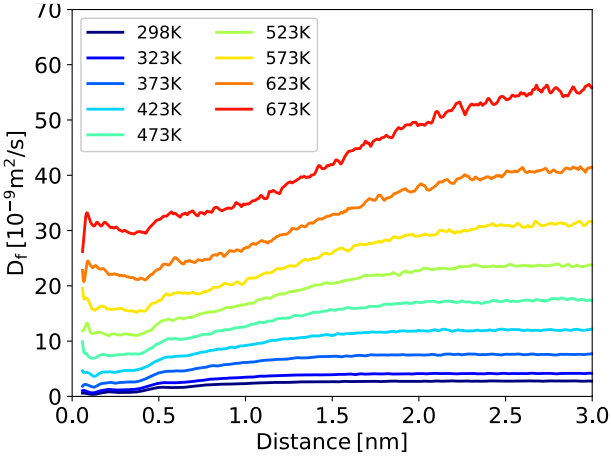
Figure S12. Schematic image of the definition of hydrogen bond [57]; the geometrical criterion related to (D) Donor, (H) Hydrogen and (A) Acceptor is $r < r_{HB} = 0.35$ nm and $\alpha < \alpha_{HB} = 30°$. r_{HB} is the range of the first coordination shell of a H_2O molecule. Hydrogen bonds break when the amplitude of the libration is about α_{HB}.



(a) 0.1 MPa



(b) 10 MPa



(c) 50 MPa

Figure S13. Self-diffusion coefficient of H_2O molecules vs distance from the muscovite surface.