

Effects of Water on the Stochastic Motions of Propane Confined in MCM-41-S Pores

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Supplementary Information

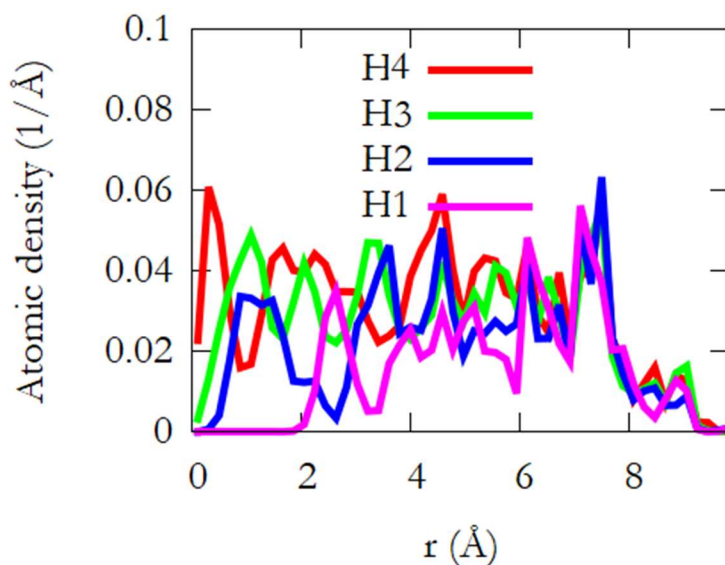


Figure S1 Atomic density distribution of Oxygen atoms in water molecules in a model MCM-41-S pore along the radial directions. Lines with different colors represent different systems as tabulated in Table 1 of the main manuscript. H1 is the system with lowest water content while water content is progressively higher in the systems H2, H3 and H4.

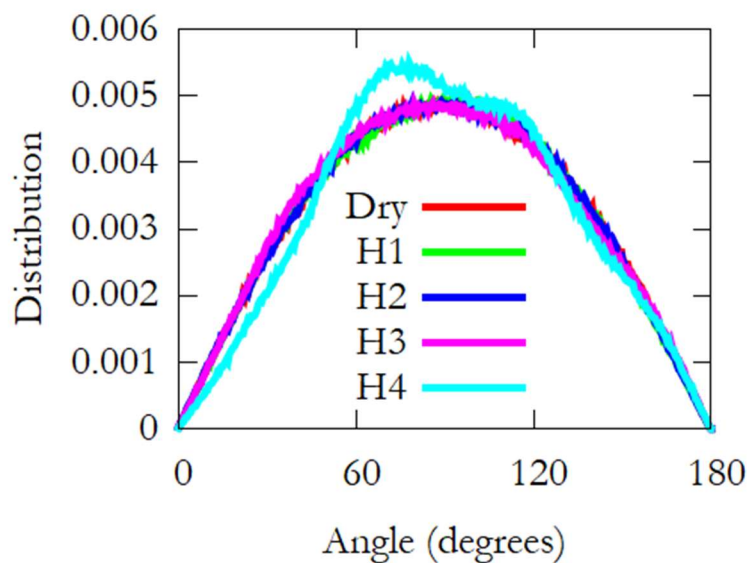


Figure S2. Distribution of the angles formed by the $\text{CH}_3\text{-CH}_2$ vector of a propane molecule with the radial direction in the model MCM-41-S pore for different systems as tabulated in Table 1. The distribution deviates from isotropic at highest water content (H4).

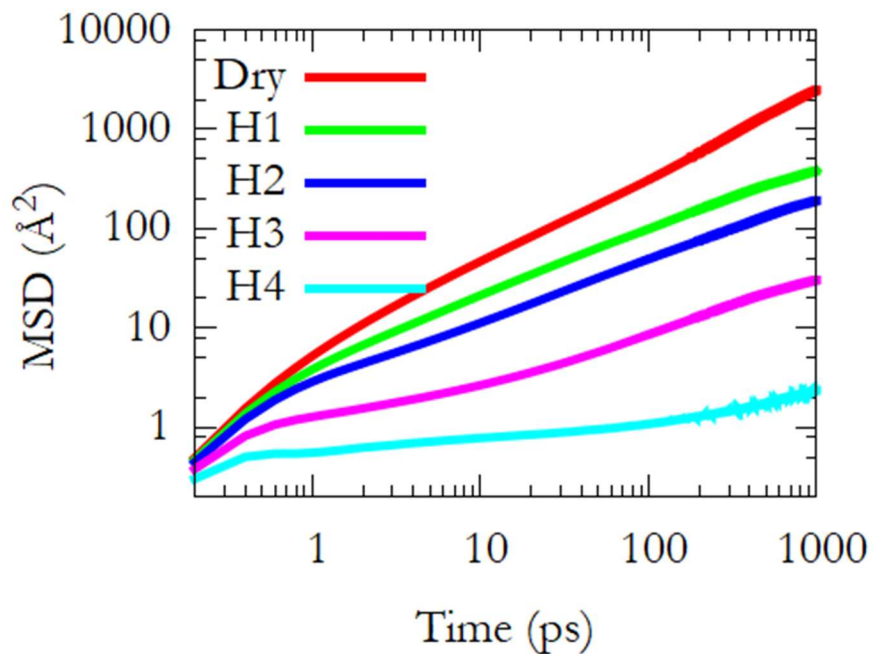


Figure S3. Mean squared displacement of the center of mass of propane molecules in model MCM-41-S pore with different moisture contents at 250 K.

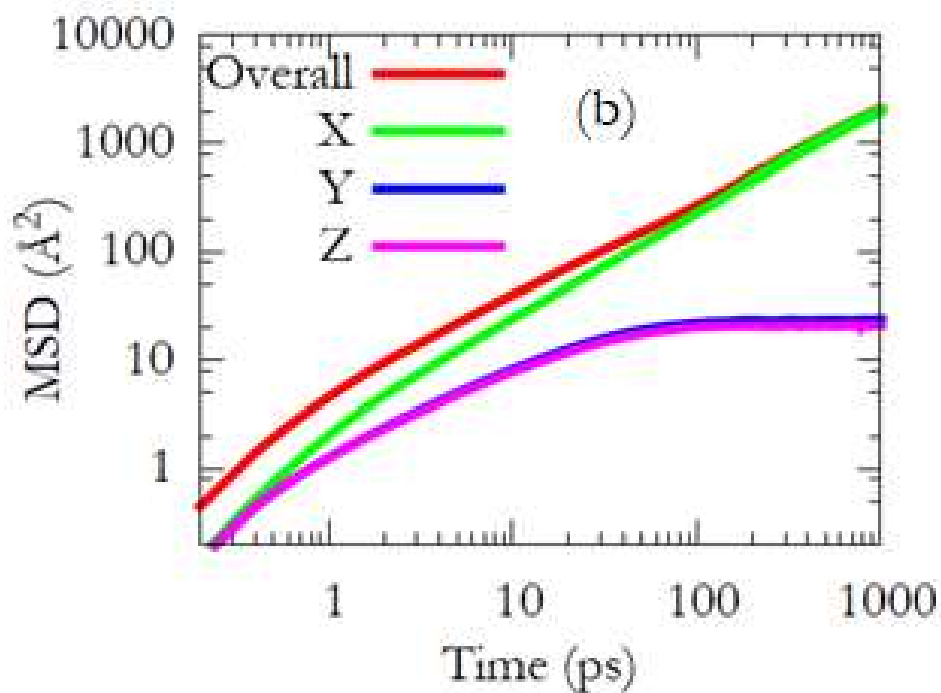


Figure S4 MSD of the dry sample at 230 K resolved along different Cartesian directions.

Table S1. 1-dimensional diffusion coefficients of water in the systems listed in Table 1 of the main manuscript. For the system H4 mobility of water was severely restricted prohibiting an estimate of the diffusion coefficient.

Sample	D ($\times 10^{-10}$ m ² /s)	
	230 K	250 K
Dry	N. A.	N. A.
H1	0.11 \pm 0.02	0.14 \pm 0.02
H2	0.10 \pm 0.04	0.12 \pm 0.01
H3	0.09 \pm 0.01	0.13 \pm 0.02
H4	-	-