

Supporting Material

Effects of Pore Size on Water Dynamics in Mesoporous Silica

Steven A. Yamada,[†] Samantha T. Hung,[†] Ward H. Thompson,^{‡*} and Michael D. Fayer^{†*}

[†]Department of Chemistry
Stanford University, Stanford, CA 94305, USA
*Phone: (650) 723-4446; Email: fayer@stanford.edu

[‡]Department of Chemistry
University of Kansas, Lawrence, KS 66045, USA
*Phone: (785) 864-3980; Email: wthompson@ku.edu

I. Figures

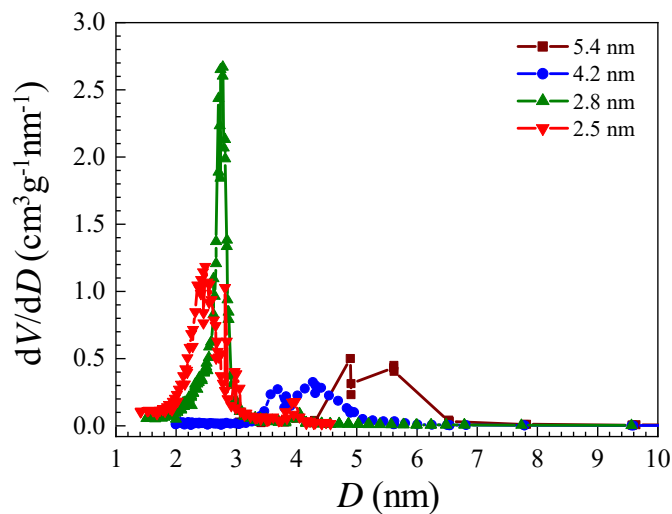


Figure S1. Pore diameter distributions, obtained as previously described,^{1,2} for the silica samples used in this work.

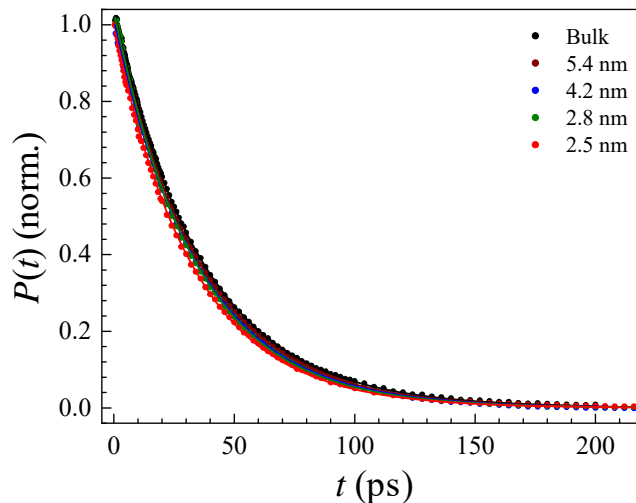


Figure S2. Isotropic pump-probe signal decays near the band center (2075.6 cm^{-1}) as a function of pore size. The time constants of the single exponential decays correspond to the SeCN^- CN stretch vibrational lifetimes.

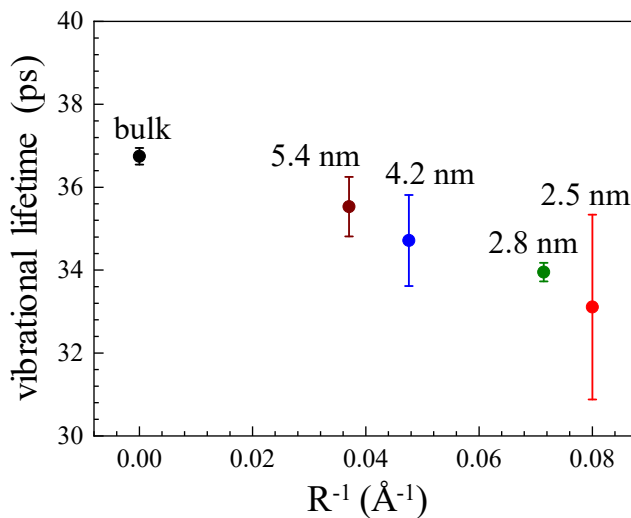


Figure S3. Vibrational lifetime of the SeCN^- CN stretch as a function of the reciprocal pore radius.

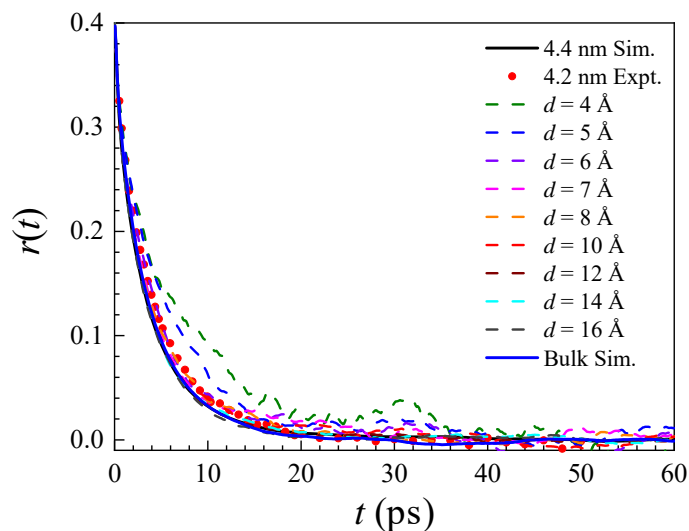


Figure S4. Simulated $r(t)$ analyzed as a function of the distance between the C atom and nearest pore O atom, d , for the 4.4 nm silica pore. The measured data for the 4.2 nm pore (red points) are shown for comparison. This figure is essentially the same as Fig. 10a, but with enhanced spatial resolution.

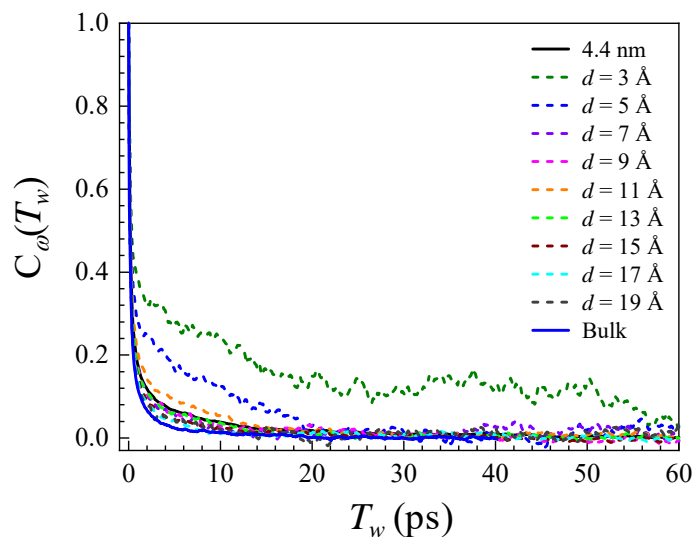


Figure S5. Simulated normalized FFCF as a function of the distance, d , between the C atom and nearest pore O atom (dashed curves) compared to the total normalized FFCF for the 4.4 nm model pore (black solid curve) and bulk solution (blue solid curve). This figure is essentially the same as Fig. 12a, but with enhanced spatial resolution.

References

- (1) Barrett, E. P.; Joyner, L. G.; Halenda, P. P. The Determination of Pore Volume and Area Distributions in Porous Substances. I. Computations from Nitrogen Isotherms. *J. Am. Chem. Soc.* **1951**, *73*, 373.
- (2) Yamada, S. A.; Shin, J. Y.; Thompson, W. H.; Fayer, M. D. Water Dynamics in Nanoporous Silica: Ultrafast Vibrational Spectroscopy and Molecular Dynamics Simulations. *J. Phys. Chem. C* **2019**, *123*, 5790.