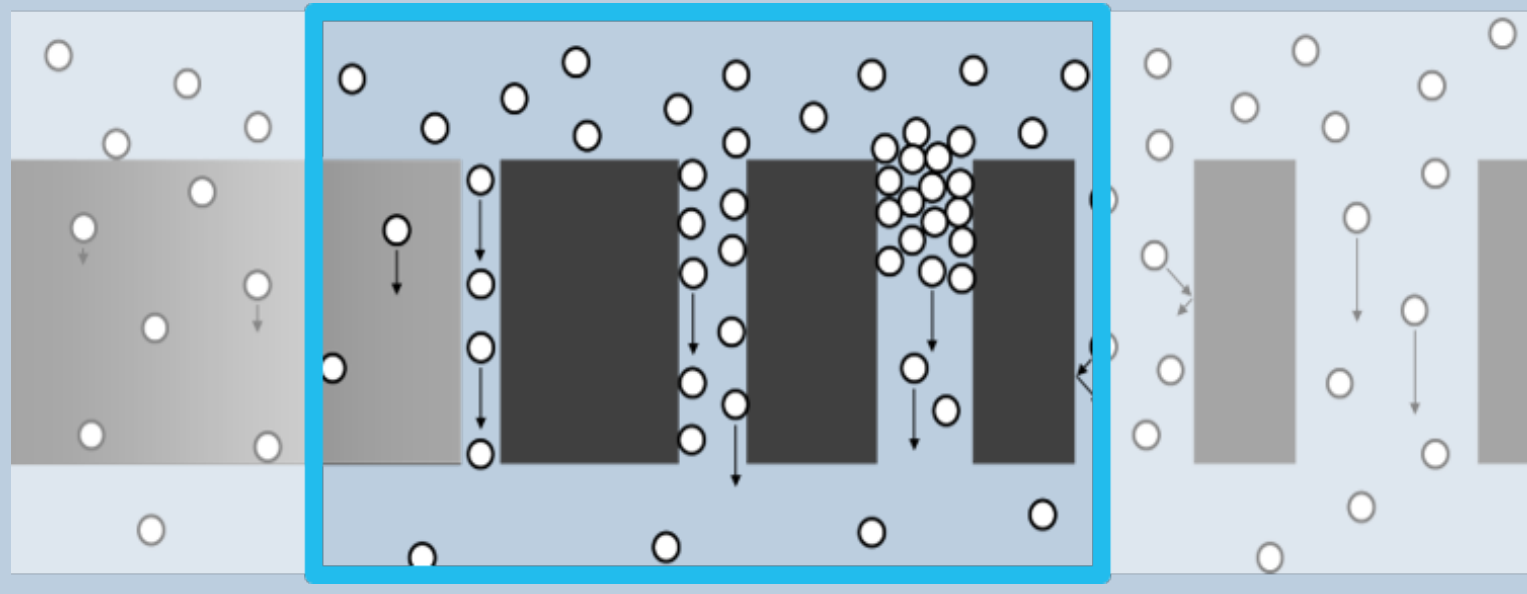# Impact of Hydrophobicity on Structure and Dynamics inside Nanopores

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Discover Nanopores

Figure 1: We are studying nanopores < 2 nm in diameter. Diffusion is a mixture of surface, configurational and capillary effects.

Materials and Methods
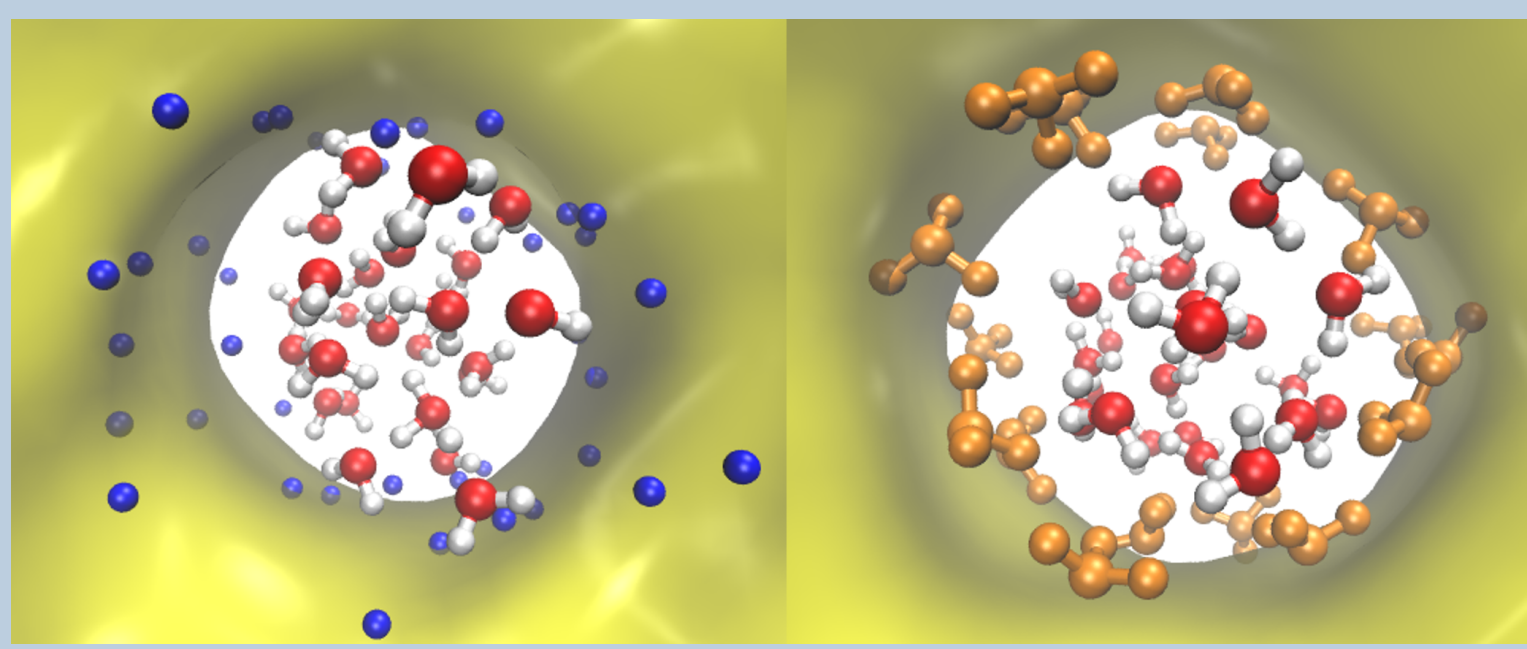
Figure 2: Abstracted silica oxide pore systems with functional groups and water depicted on a molecular level. Pristine hydrophilic (left) and hydrophobic trifluoromethyl (right).

$$X_{abc}^{res,(2)}(\omega) = \frac{Q(\omega)}{i\omega^2} \int_0^\infty dt e^{-i\omega t}$$
$$\times \left\langle \sum_{i,j} g_t(r_{ij}(0); r_t \dot{r}_{c,i}^{OH}(0) \frac{r_j^{\vec{OH}}(t)\dot{\vec{r}}_j^{OH}(t)}{|\vec{r}_j^{OH}(t)|} \right\rangle,$$

$$if \ a = b, \ else \ X_{abc}^{res,(2)}(\omega) = 0.$$

Formalism to calculate the SFG Spectra from velocity-velocity ACF. Results are surface specific and sensitive to orientation.

Conclusion
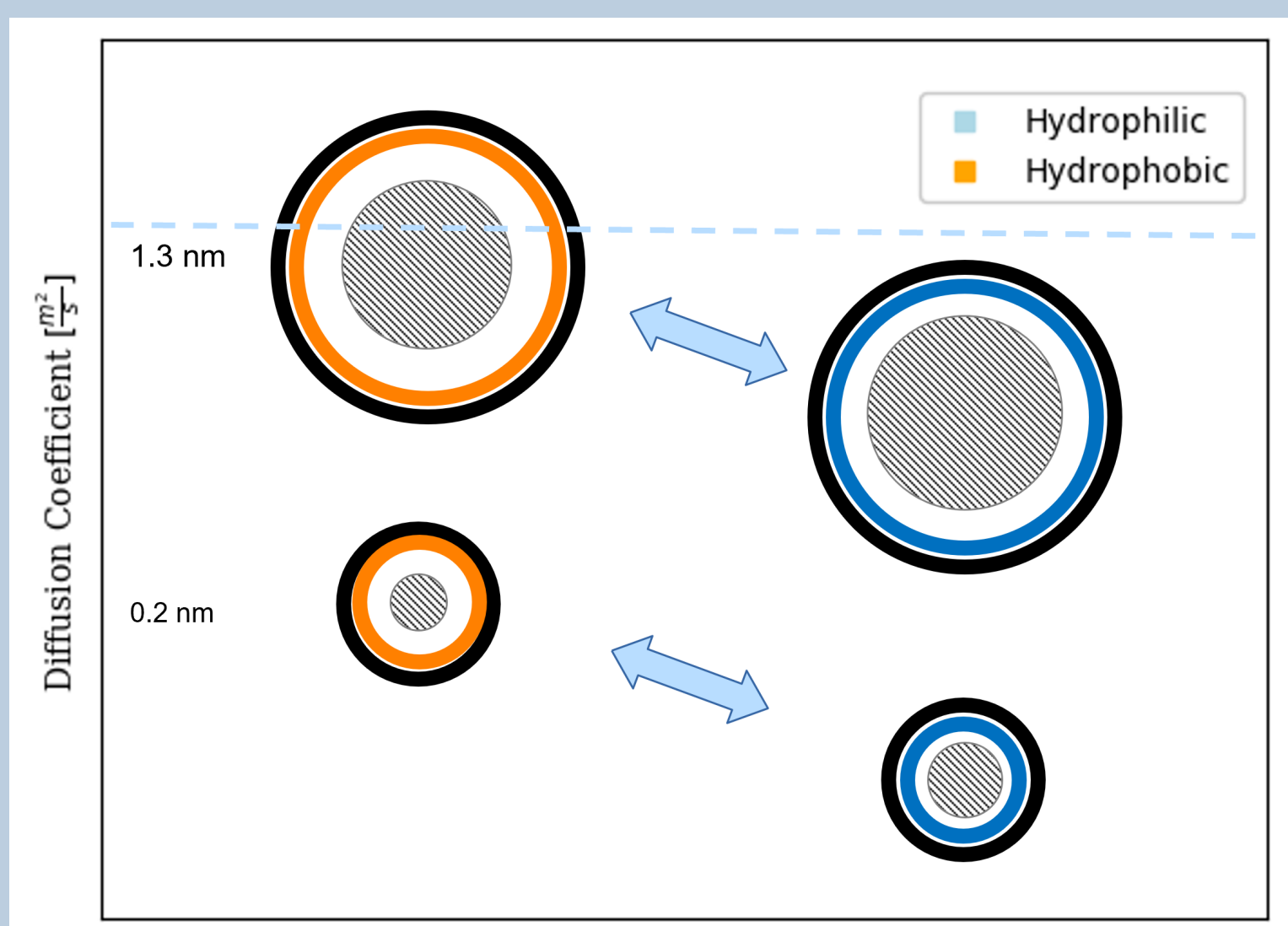
Figure 3: Generally diffusion increases with bigger pore sizes. The distance between hydrophobic pore walls and water is larger than in the hydrophilic cases. Water diffusion in hydrophobic pores is faster for comparable pore sizes, even higher than in bulk water for larger hydrophobic pores.
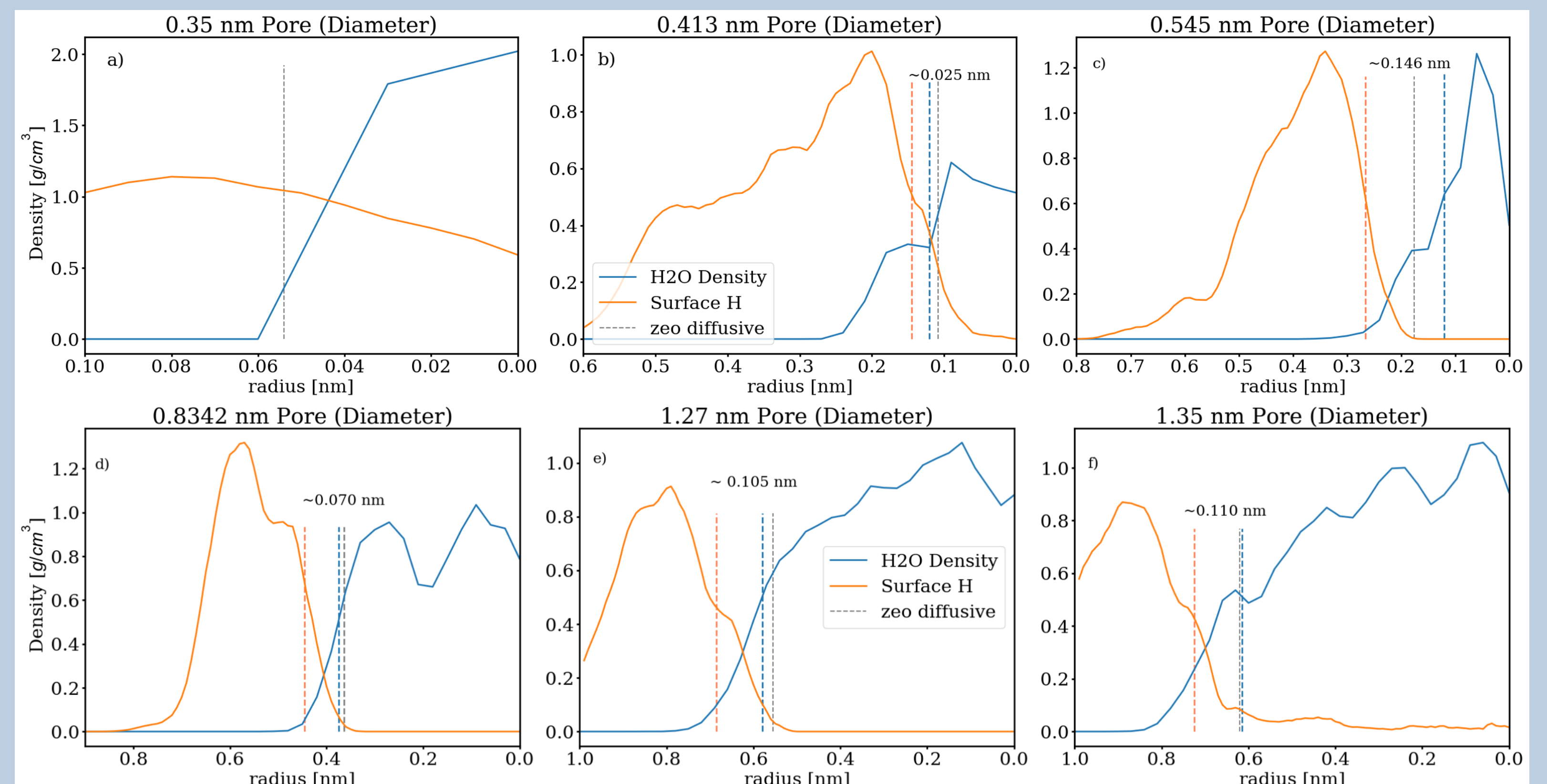
References

[1] Christian Weinberger, Frederik Zysk, Marc Hartmann, Naveen K Kaliannan, Waldemar Keil, Thomas D Kühne, and Michael Tiemann. The structure of water in silica mesopores–influence of the pore wall polarity. *Advanced Materials Interfaces*, 9(20):2200245, 2022.

Acknowledgements

PC² Paderborn Center for Parallel Computing

Density and Structure

Figure 4: The radial density of water (blue) and functional wall elements (orange) for the pristine pores from the smallest pore system (a) to the largest one (f). The density is shown from the pore surface towards the center of the pore. The Gibbs dividing surfaces are indicated as lines and their distance is shown.
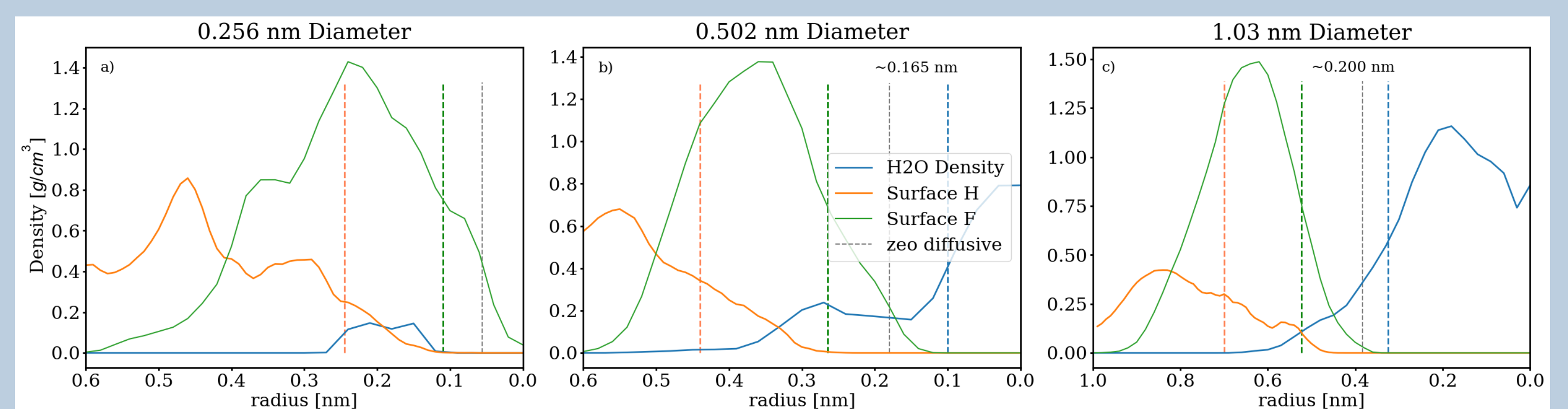

Figure 5: The radial density of water (blue) and functional wall elements H (orange) and F (green) for the hydrophobic pores from the smallest pore system (a) to the largest one (c).

Dynamics and Correlation with Structure
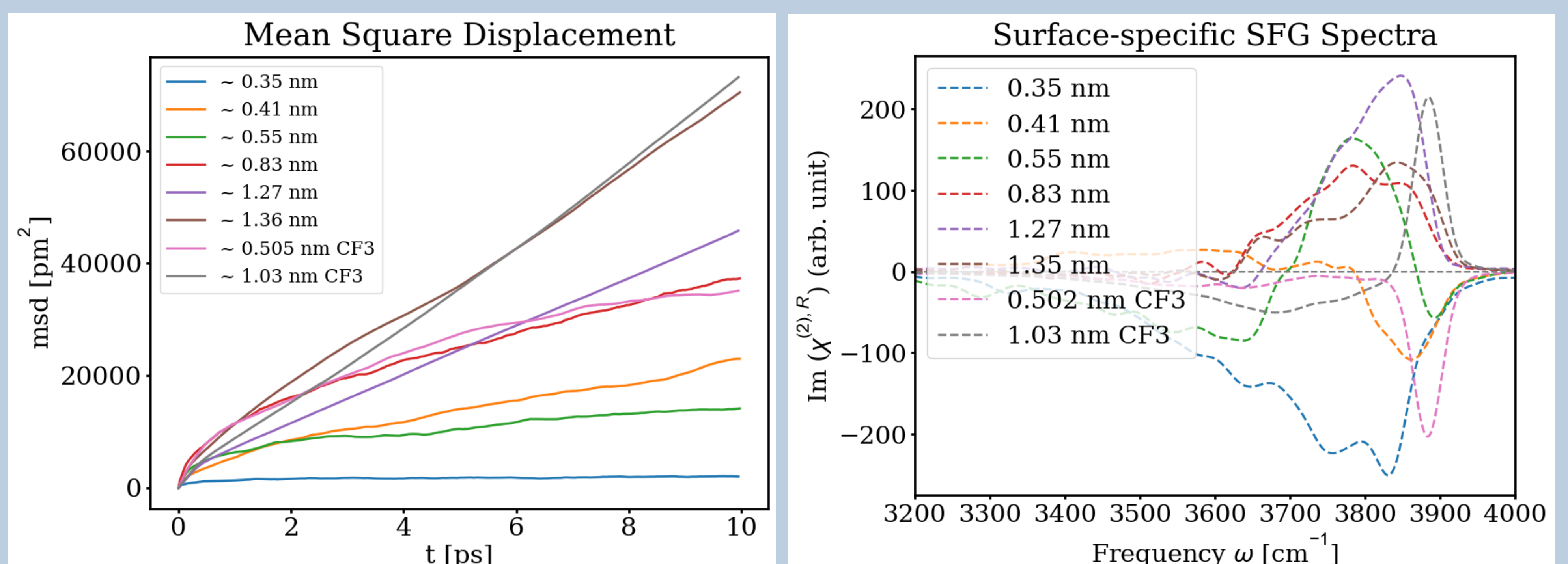
Figure 6: Diffusion calculated by mean square displacement for all pristine pore systems and two hydrophobic ones. For comparable sizes diffusion in hydrophobic pores is higher (left).; Imaginary part of the SFG response. Positive values mean water is oriented towards the pore surface, while negative values represent overrepresentation of water oriented away from the surface (right).
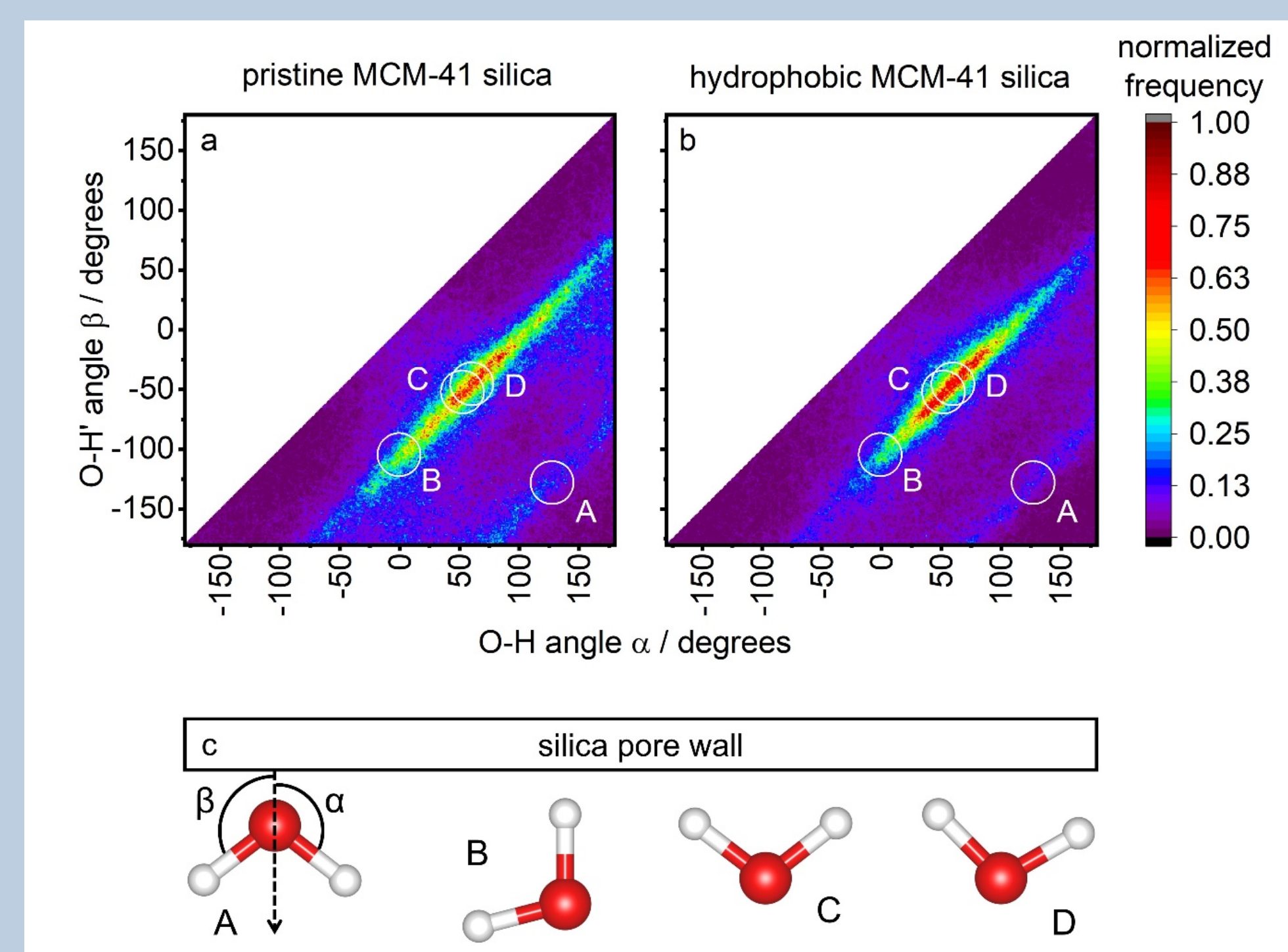
Figure 7: Exemplary analysis of angular distribution of the water molecule's OH stretchingmodes relative to the hydrophilic (pristine) (a) and hydrophobic silicasurface (b). Example water molecule configurations are depicted in (c). Generally more configurations of type C and D in hydrophilic systems and A in hydrophobic systems. Full analysis in ref. [1].