

Electronic Supplementary Information (ESI) for

Impact of Surface Wettability on Dynamics of Supercooled Water Confined in Nitrogen-Doped Ordered Mesoporous Carbon

Clinton G. Wiener,^{a, ‡, †} Zhe Qiang,^{a, ‡, †} Yanfeng Xia,^b Madhusudan Tyagi,^c and Bryan D. Vogt^{a, *}

^a Department of Polymer Engineering, University of Akron, Akron, OH, 44325, USA

^b Department of Polymer Science, University of Akron, Akron, OH, 44325, USA

^c Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, MD, 20899, USA and Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742 USA

[†] Present address: 3M, Center St., St. Paul, MN, 55144 (C.G.W.)

Department of Chemical and Biological Engineering, Northwestern University, Evanston, IL, USA, 60208 (ZQ)

[‡] These authors contributed equally.

* To whom correspondence should be addressed: vogt@uakron.edu (B.D.V.)

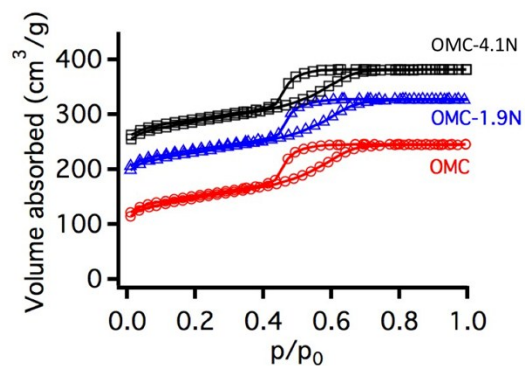


Figure S1. Adsorption-desorption isotherms of OMC, OMC-1.9N and OMC-4.1N. The isotherms of OMC-1.9N and OMC-4.1N has been vertically offset by 100 cm³/g and 150 cm³/g

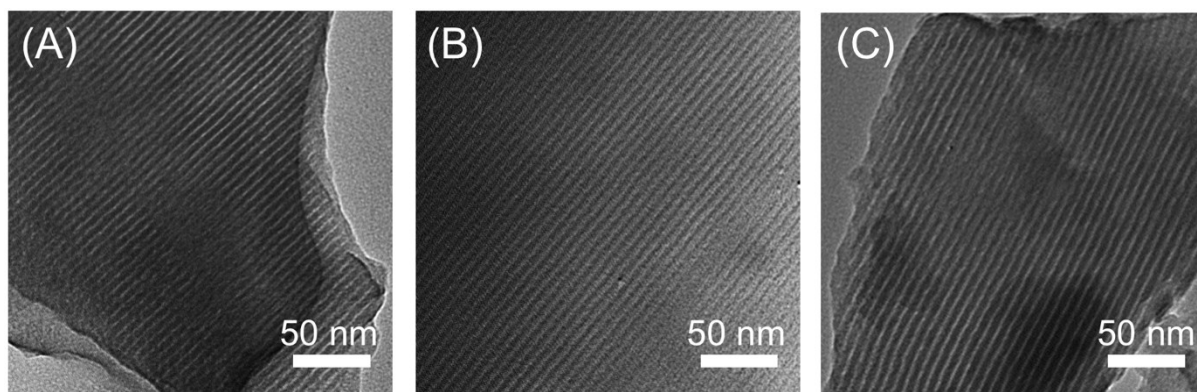


Figure S2. TEM images of (A) OMC; (B) OMC-1.9N and (C) OMC-4.1N

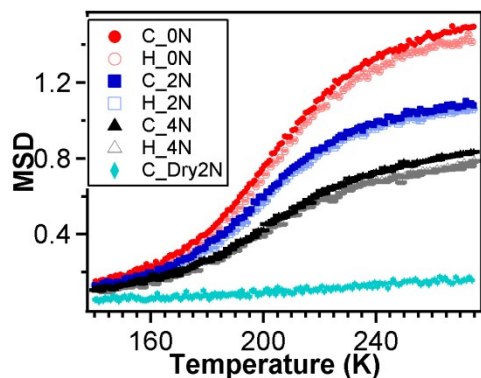


Figure S3. MSD results for cooling rate of 0.8K/min from room temperature to 4K and then reheating at 2K/min. Similar trends in sample, with the more hydrophobic 0N sample showing the most mobility. The legend denotes whether the MSD measured was on the cooling trend (C) or heating trend (H) for the 0%N, 1.9%N, and 4.1%N.

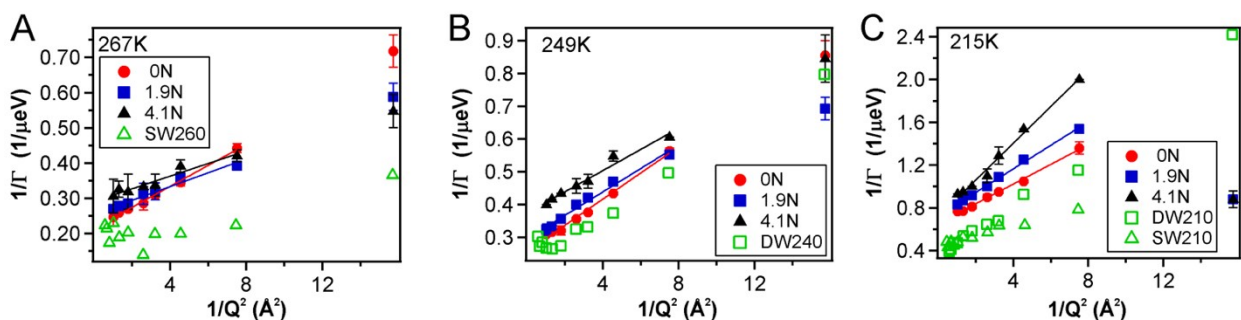


Figure S4. Linear regression of $1/\Gamma$ as a function of $1/Q^2$ for different OMCs as an alternative route to determine the diffusivity of water and the time between jumps. Error bars throughout the text represent one standard deviation.

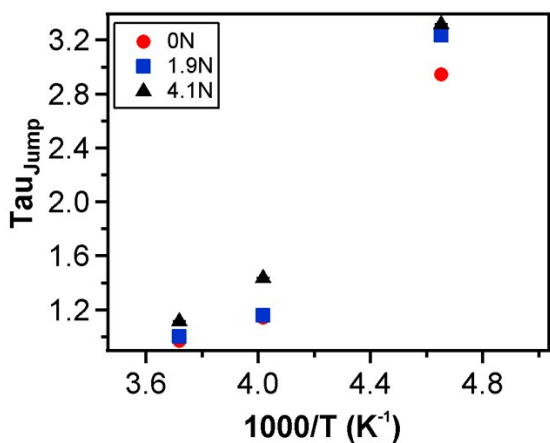


Figure S5. τ_o as a function of $1000/T$ for different OMCs. This does not appear to be Arrhenius.

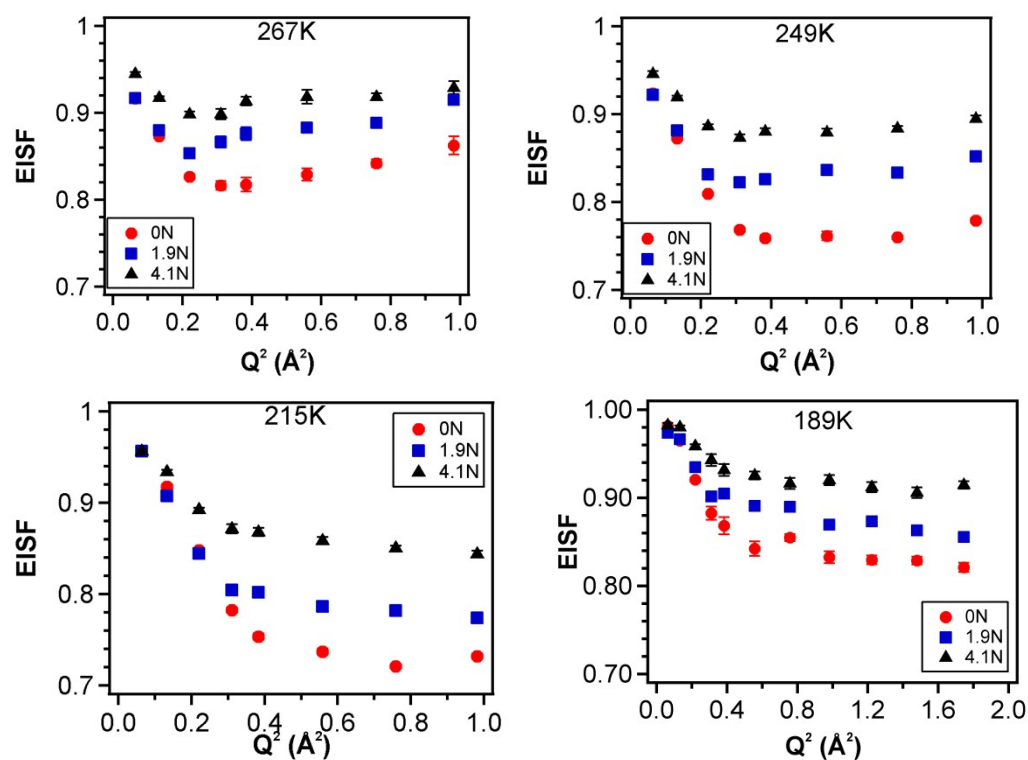


Figure S6. Elastic incoherent structure factor (EISF) calculated from Lorentzian fits of full energy window scans. Decreasing values indicate a decrease in the elastic scattering fraction of the sample. This suggests at all temperatures, the more hydrophobic OMC-0N has the largest dynamic fraction of protons, while the OMC-4.1N has the lowest fraction. This would indicate, that although the dynamics of the water remains quite similar from the FWHM trends, the fraction of water participating in the motion as measured by HFBS decreases with increasing hydrophilicity.