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On the Exceptional Negative Compressibility of Zeolitic Imidazolate Frameworks (ZIFs) and Potential Application

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Contents

- Porosimetry/Neutron Diffraction study of Negative Volumetric Compressibility of ZIFs (herein ZIF-8)
- Theoretical Restrained Molecular Dynamics (RMD) study of ZIF-8 intrusion-extrusion
- Intrusion-induced ZIF-8 structural modifications
- Insights on NVC from ITT water-bridging across pore windows

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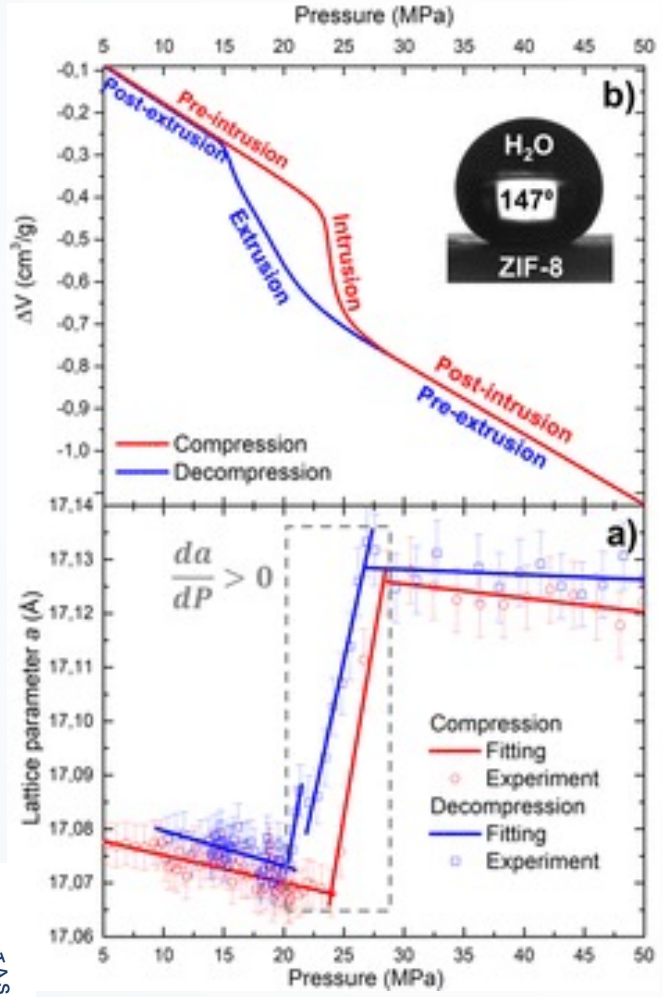
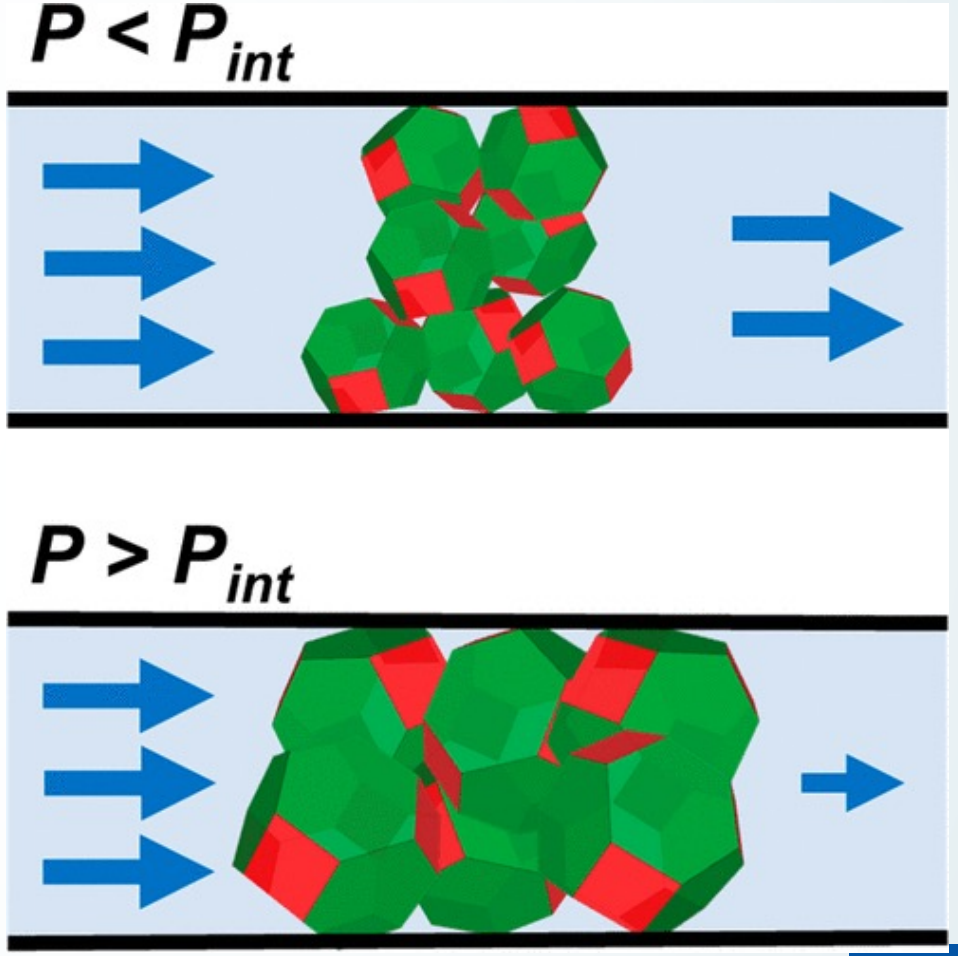
Intrusion-Extrusion ZIF-8 Porosimetry/ Neutron Diffraction Study

- Porosimetry of ZIF-8 carried out with complete intrusion-extrusion of water
- Lattice parameter measured with neutron diffraction





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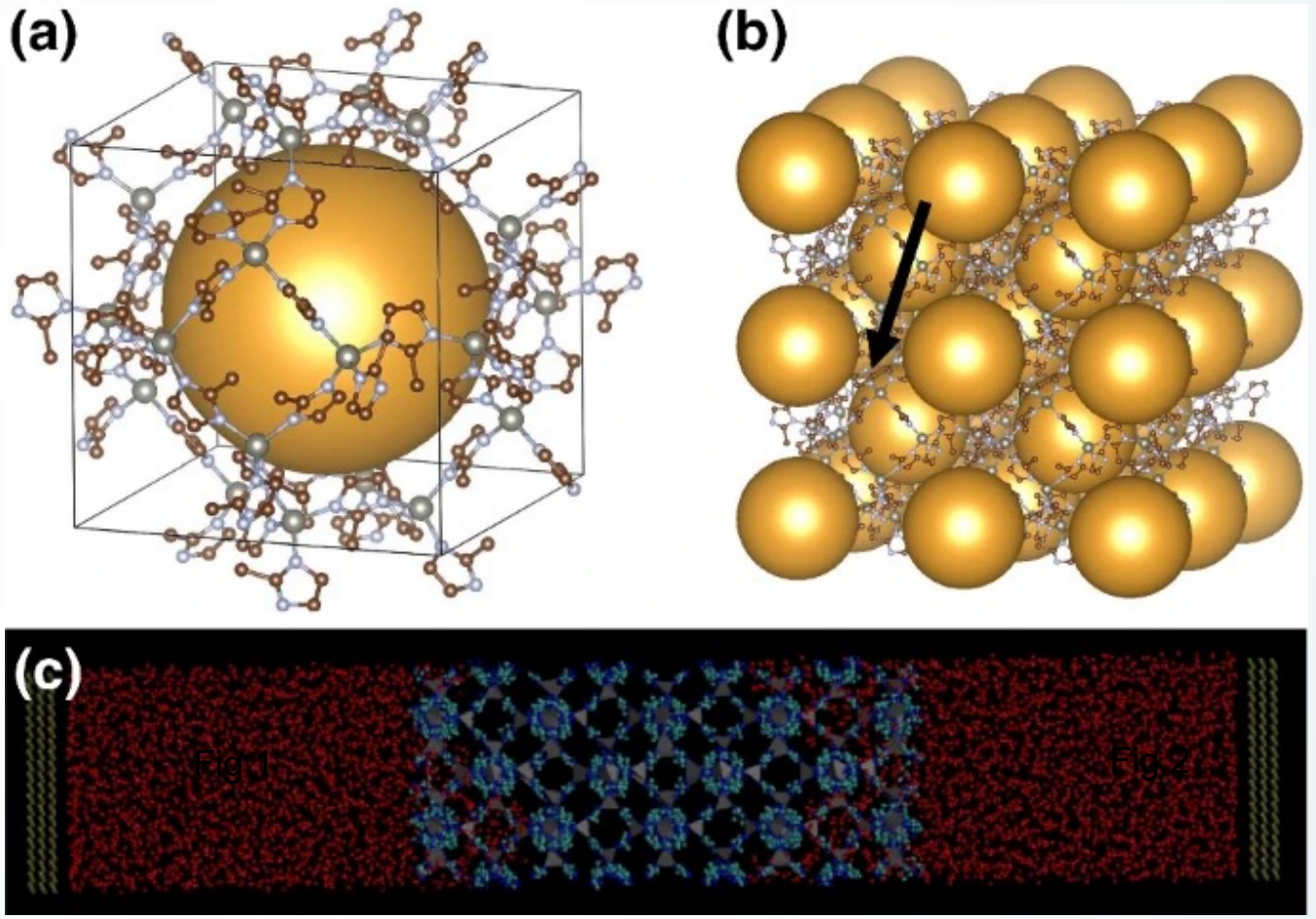
Restrained Molecular Dynamics of ZIF-8 Intrusion-Extrusion

- RMD carried out at 0-120% filling of 4x7-pore ZIF-8 slab
- Overcomes time-scale mismatch between experimental intrusion (O(10-100s)) and MD (O(1ns))



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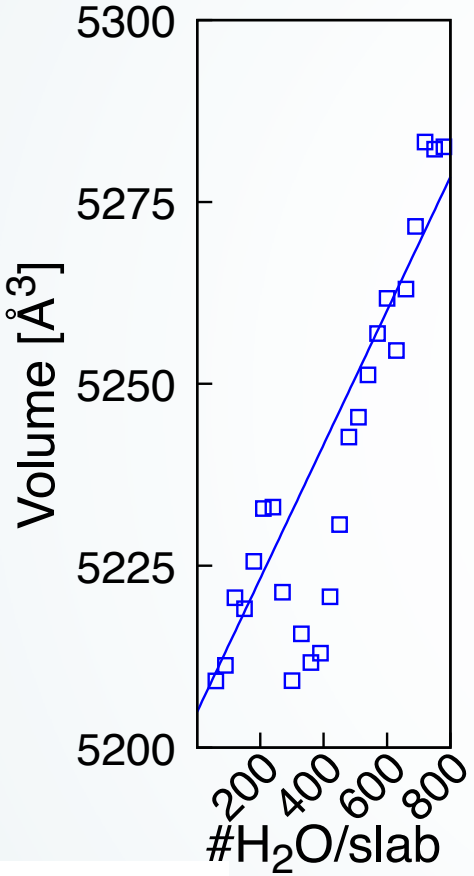
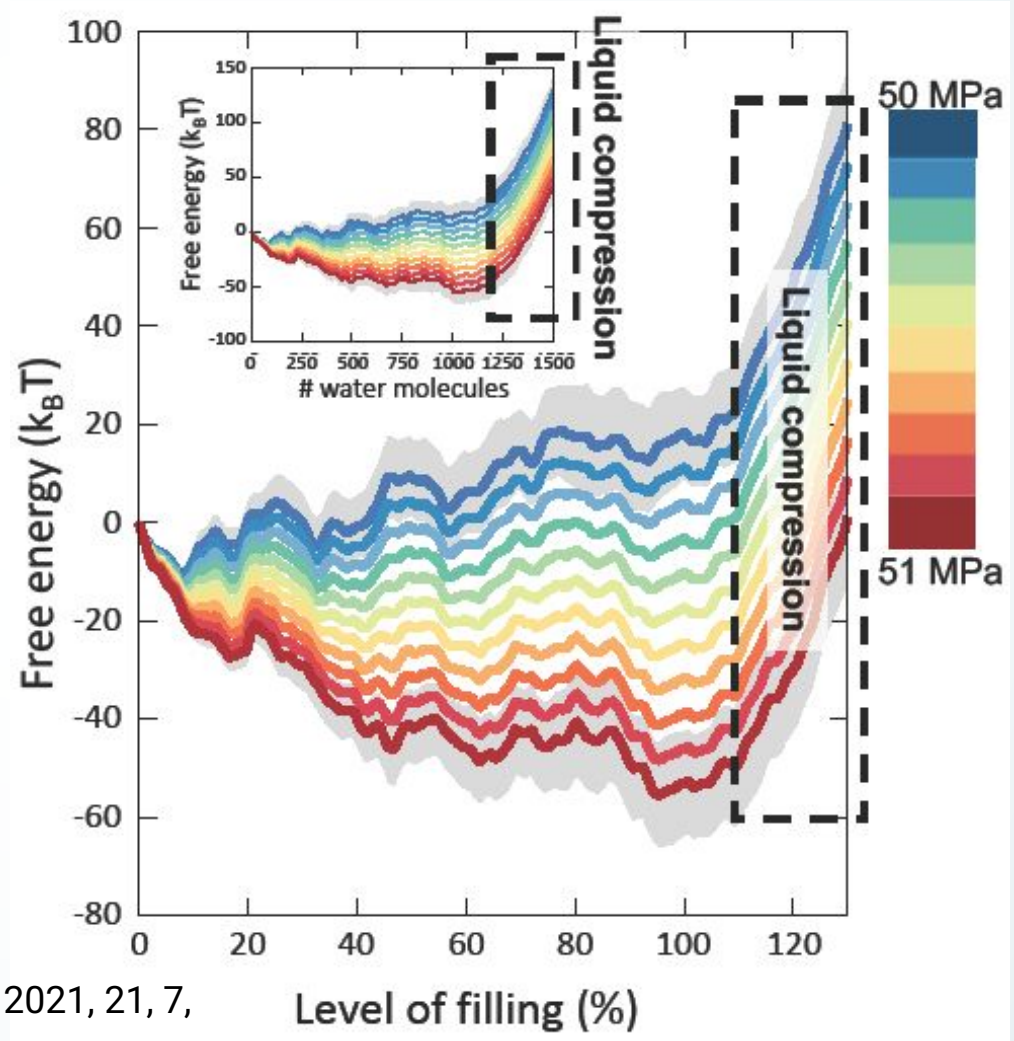
Predicted Volume Expansion and Free-Energy Profile





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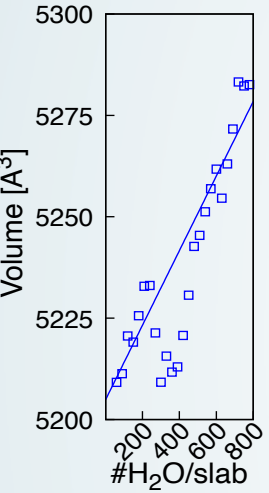
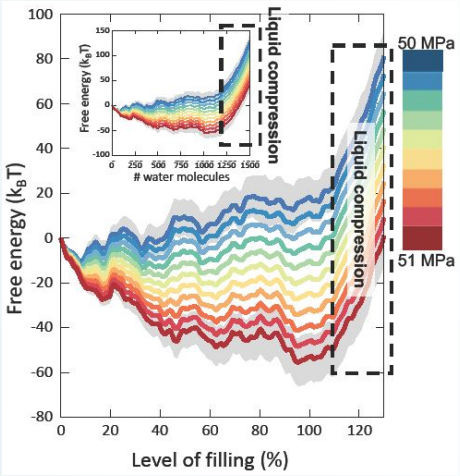
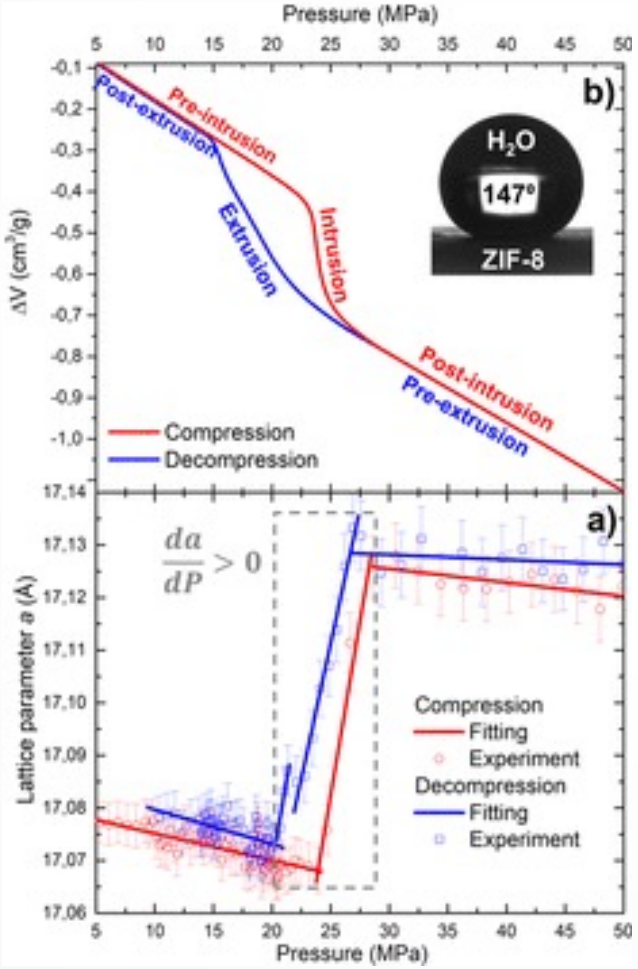
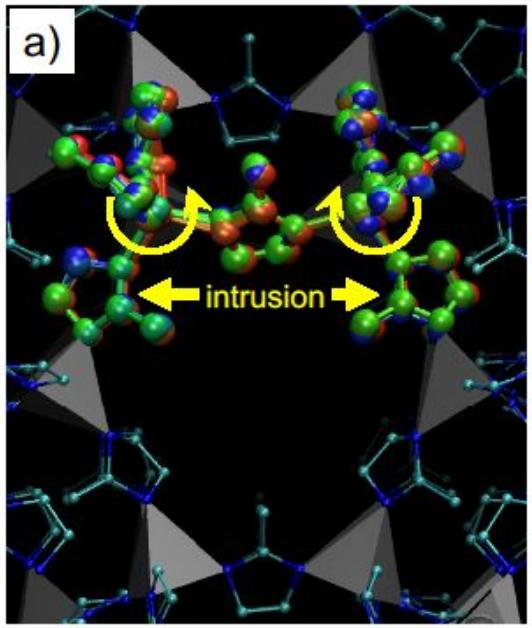
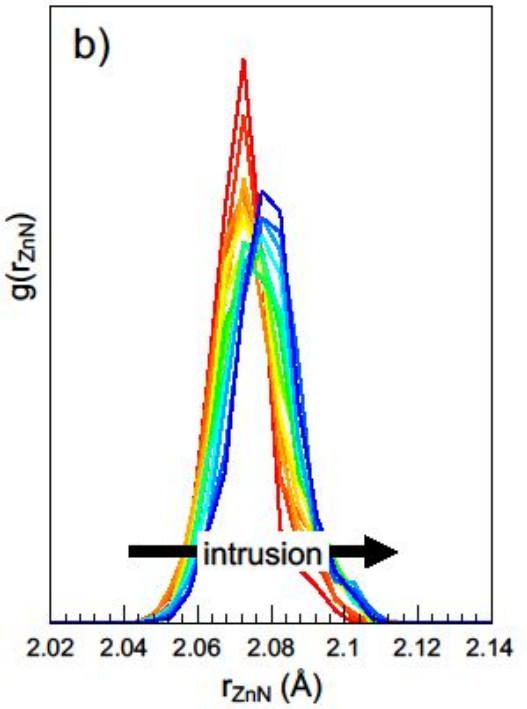
Intrusion-Induced ZIF-8 Structural Modifications











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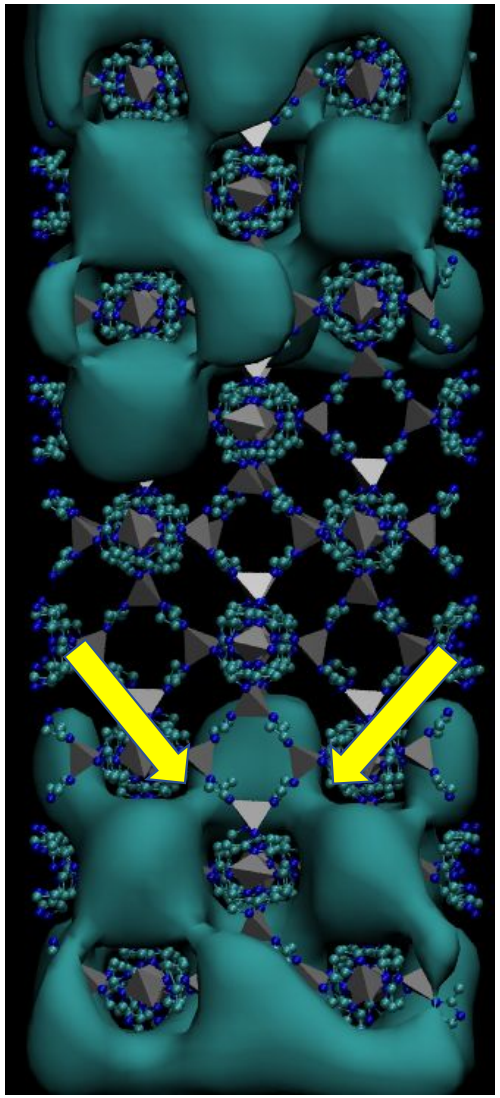
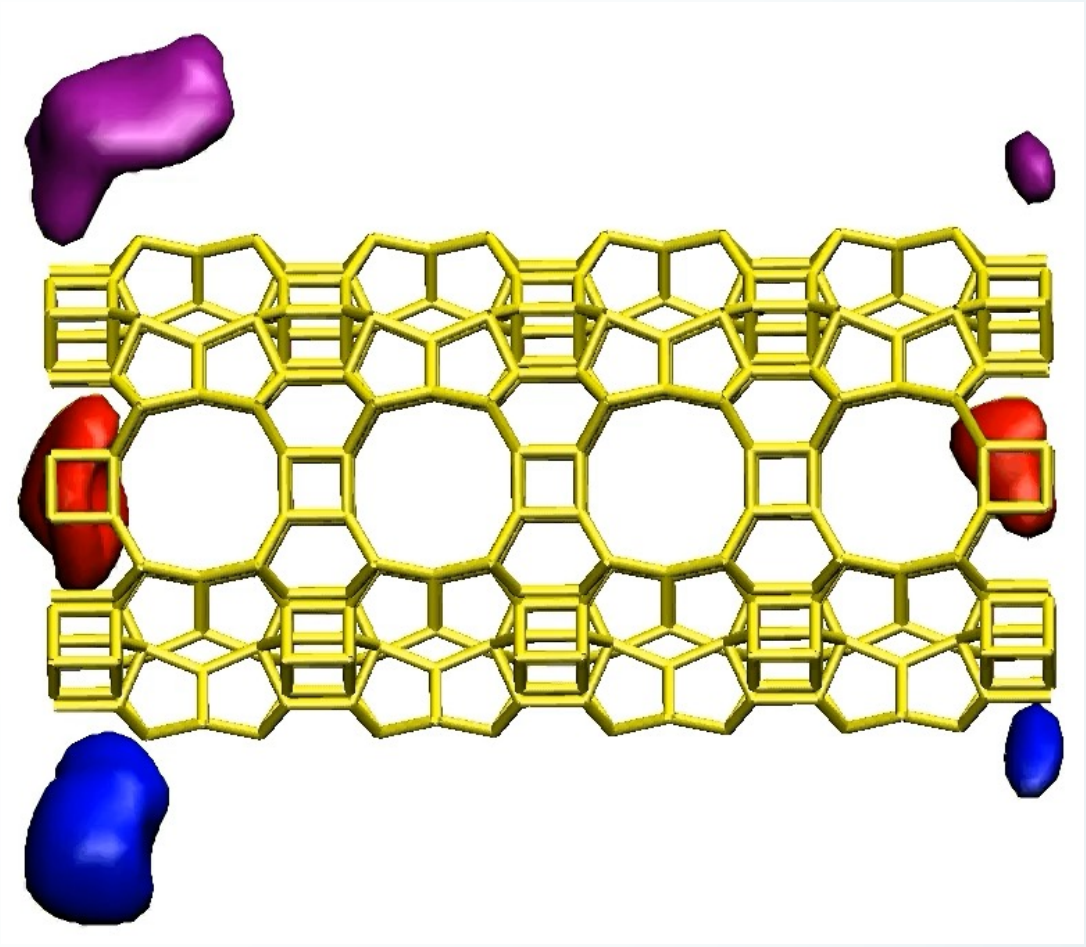
Perspectives from ITT Water-Bridging across Pore Windows

- Recently looked at the characteristics of pore-by-pore intrusion into zeolites (ITT)
- Revealed the effect of bridging pores via water in pore windows





Bushuev, Y. G. et al. *Nano Lett.* 2022, 22(6), 2164-2169.

Conclusions So Far and Future Research Direction

- ZIFs possess the highly rare property of NVC upon water intrusion.
- Theoretical RMD study reveals ZIF-8 structural modification associated with intrusion
- Potential insights from studies zeolite intrusion point to a potential explanation of ZIF-8 intrusion, currently under study
- Recently, H2020 funding was granted for the Electro-intrusion collaboration to study the viability of using ZIFs and other hydrophobic materials as nanotribolelectric generators

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Thanks for your attention!

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