



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101017858

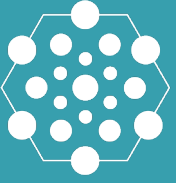
Revealing the Cage-by-Cage Mechanism of Liquid Water Intrusion into Porous Solids

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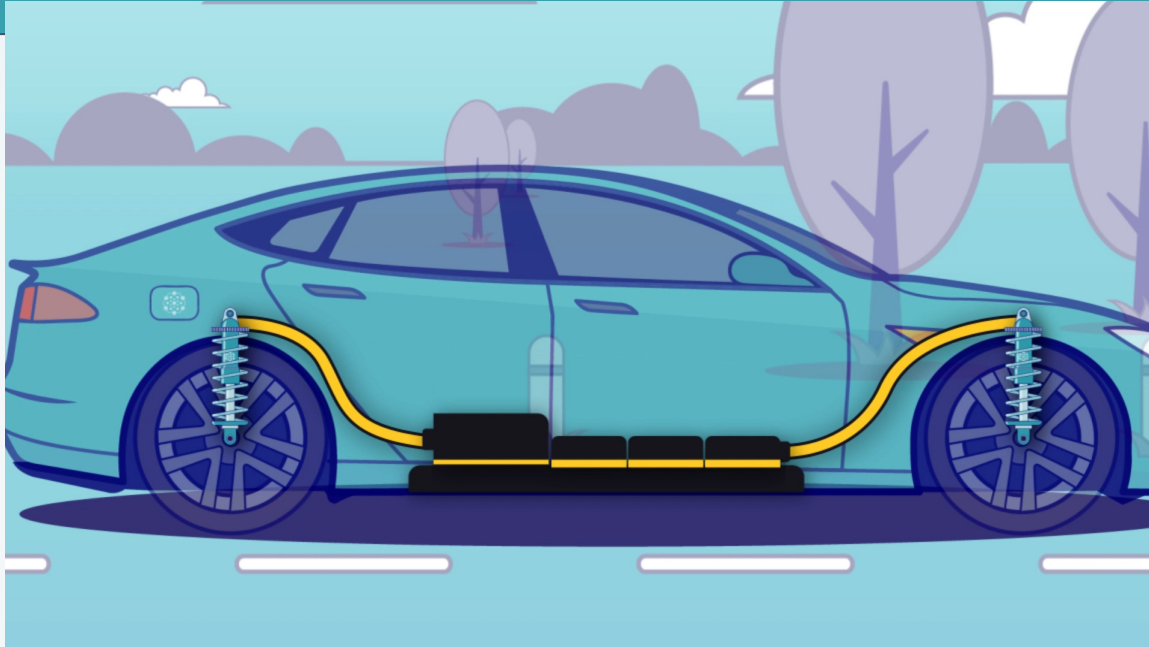
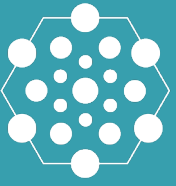


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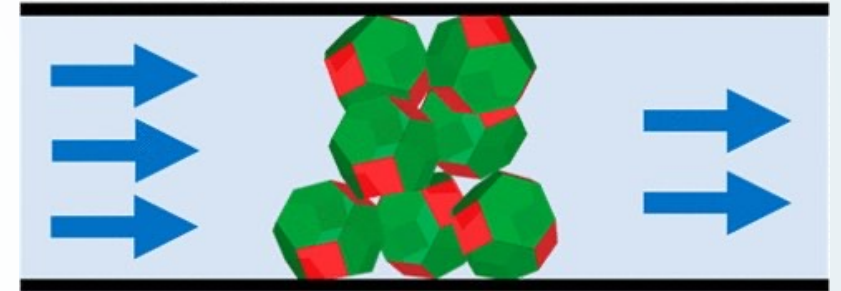


- Background on liquid-solid intrusion-extrusion applications and challenges
- ZIF-8: a potential solution?
- Unravelling the liquid intrusion mechanism into ZIF-8 via a joint theoretical-experimental approach

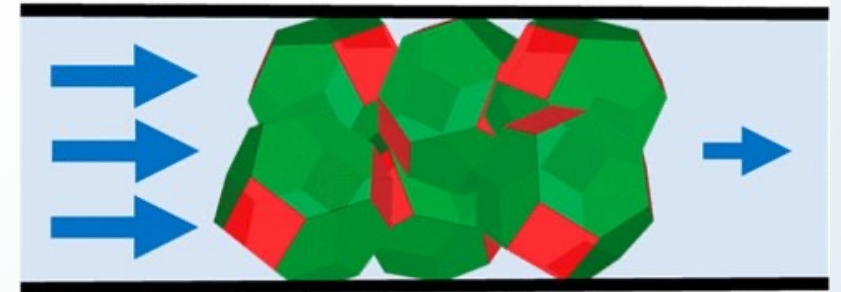
Liquid Intrusion-Extrusion: Potential Uses



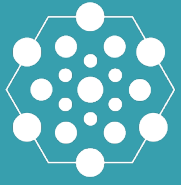
$$P < P_{int}$$



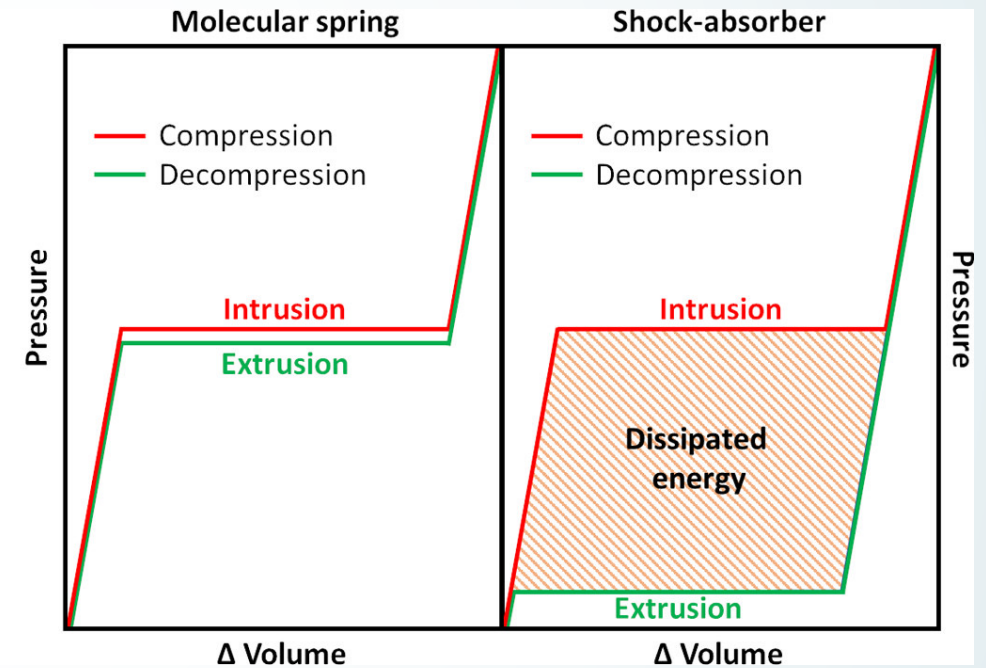
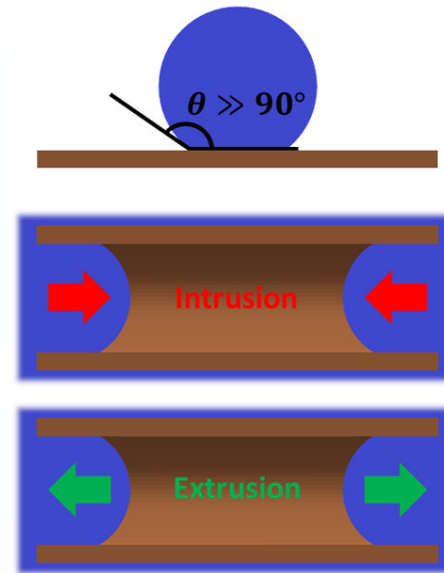
$$P > P_{int}$$



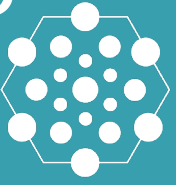
The challenges of finding suitable intruding media...



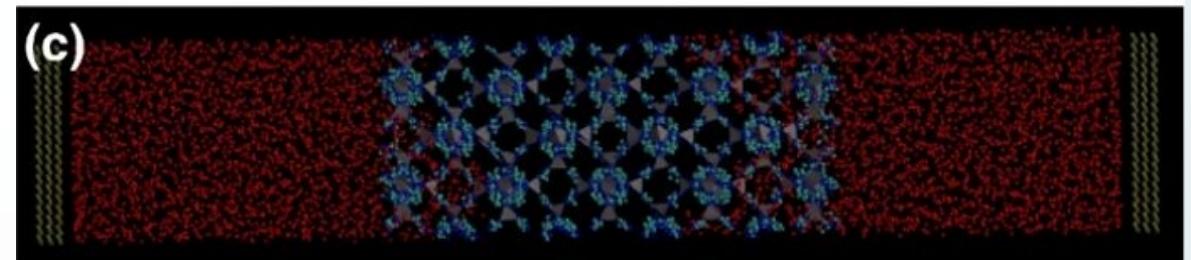
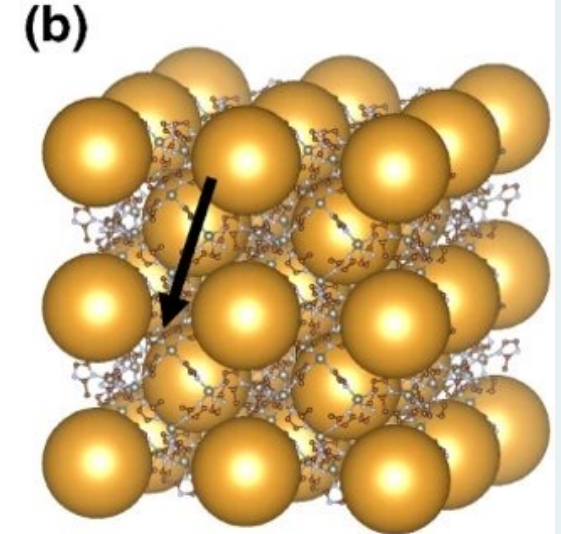
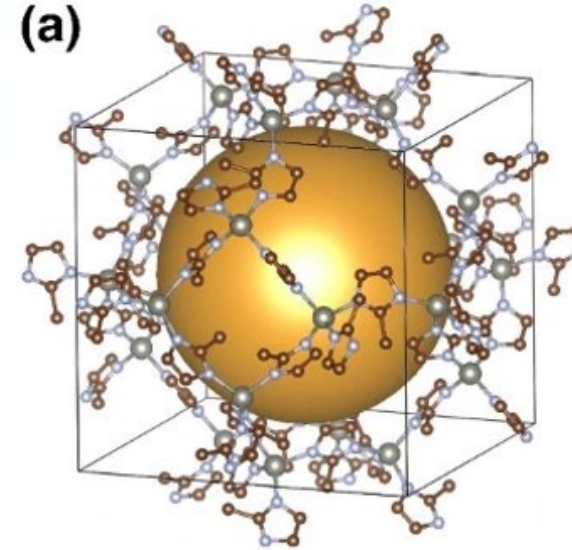
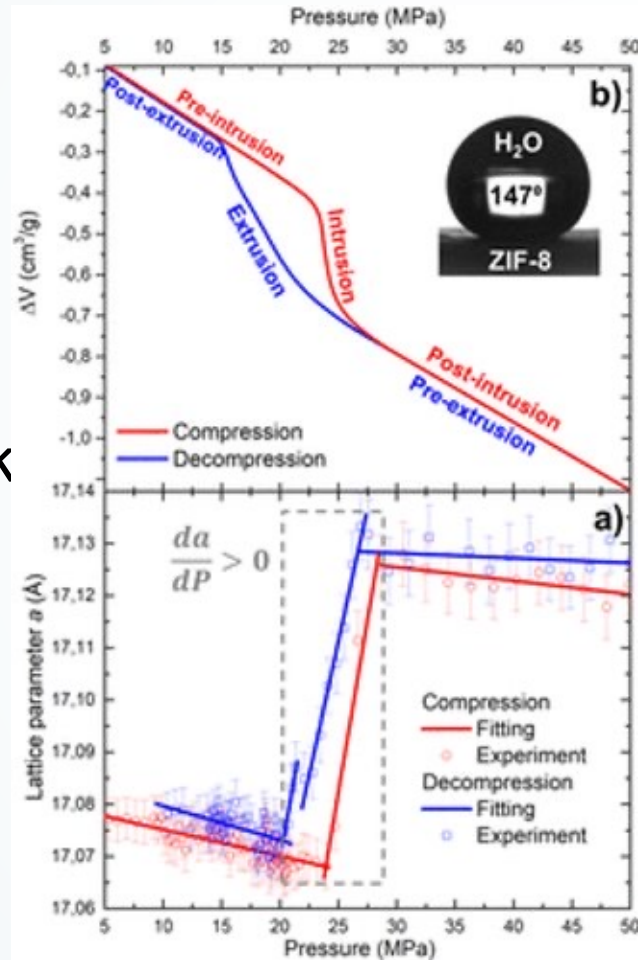
- Hydrophobic for Int-Ext cycle
- Durable for millions of cycles without performance drop
- Hysteresis (minimised = molecular spring, maximised = shock absorber)
- High energy density
- Charging (for energy recovery)



ZIF-8, the Perfect Candidate? Or How I Learned to Stop Worrying and Love Negatively Compressive Materials

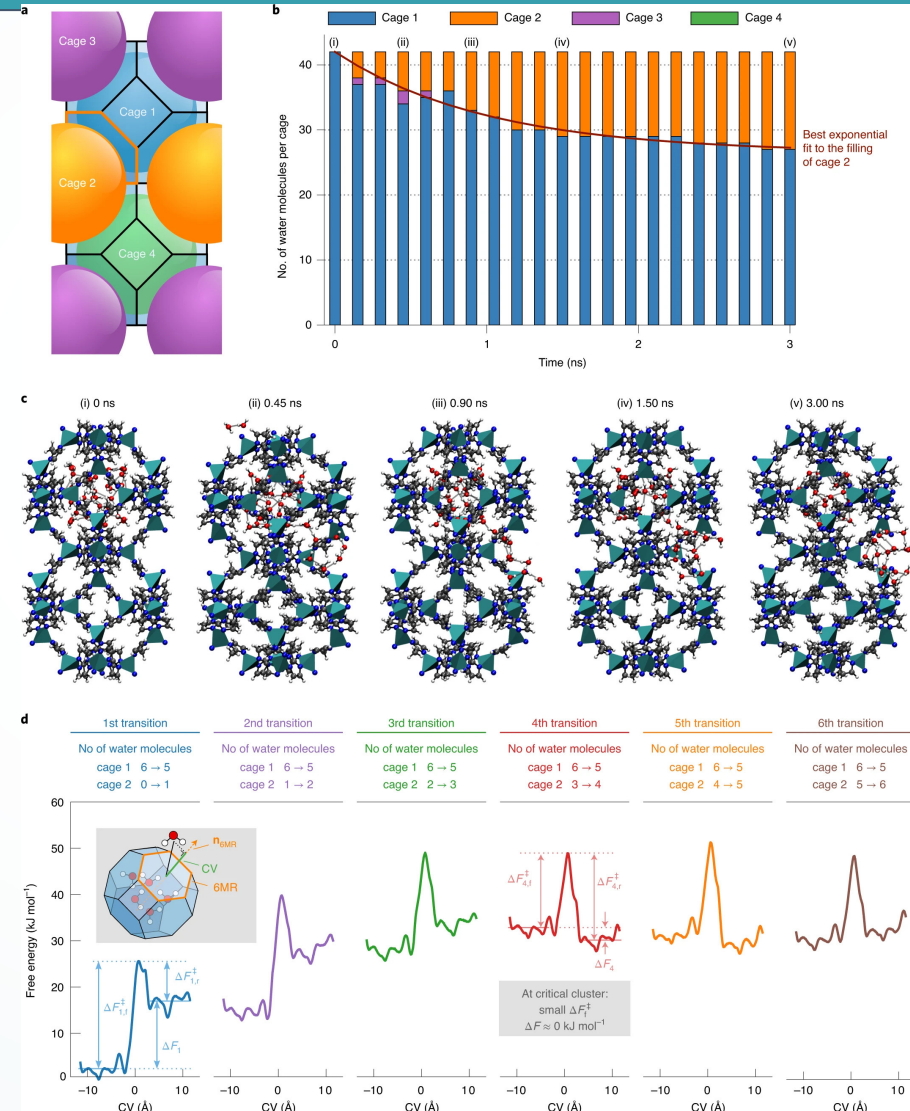
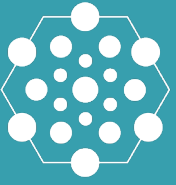


- Superhydrophobic
- Int-Ext Hysterisis
- High energy density
- Tunable framework architecture
- Large internal surface area
- Durable over int-ext cycles



Tortora et al. *Nano Lett.* 2021, 21, 7, 2848–2853

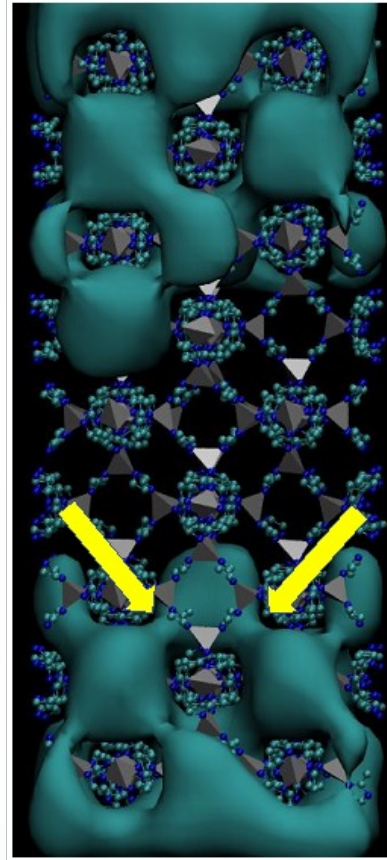
Proposed Condensation Mechanism (Sun Group)



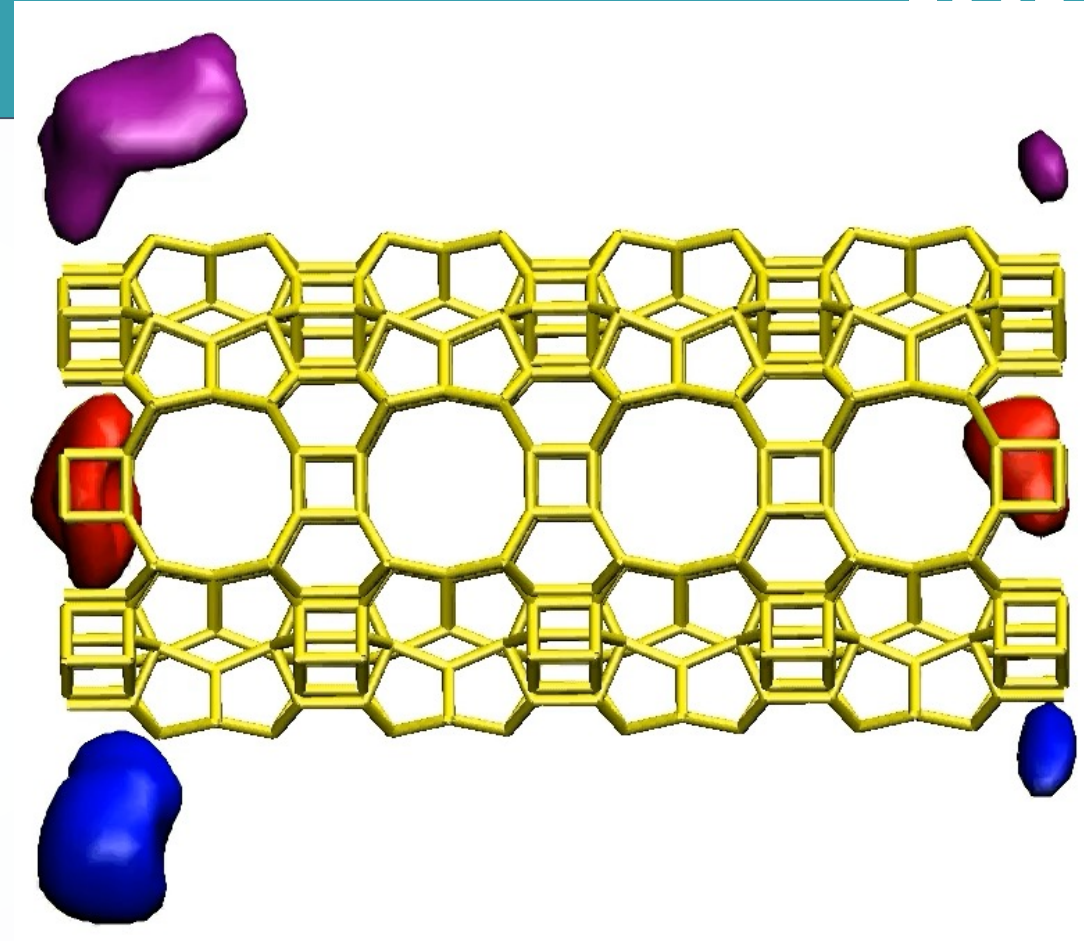
Evidence of Proposed Bridging Mechanism



- Recently looked at the characteristics of intrusion into zeolites (ITT) with bridging in lateral windows connecting channels
- Bridging pores via water in pore windows in ZIF-8 observed in previous studies

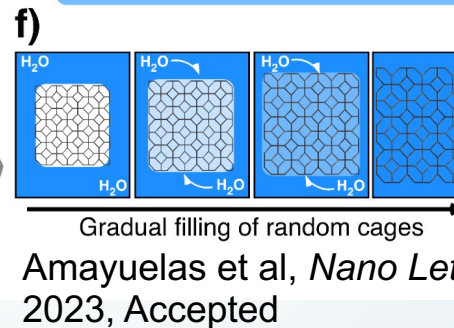
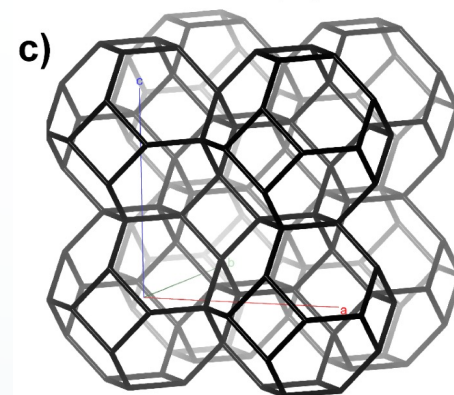
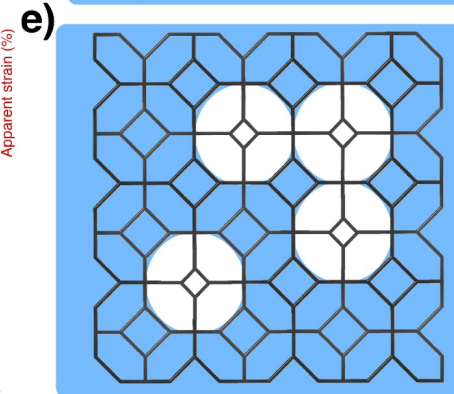
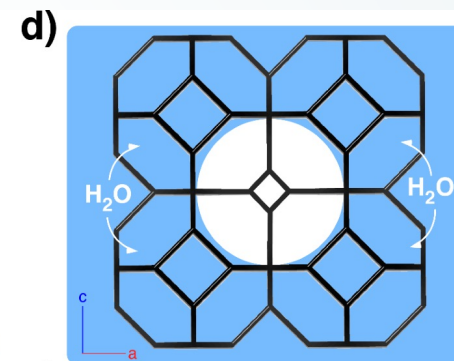
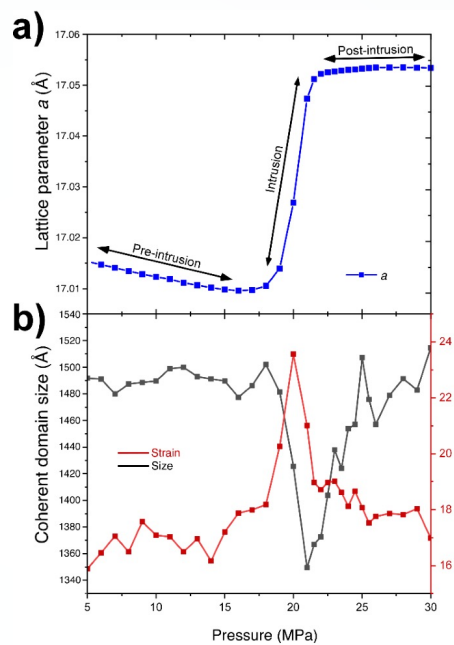
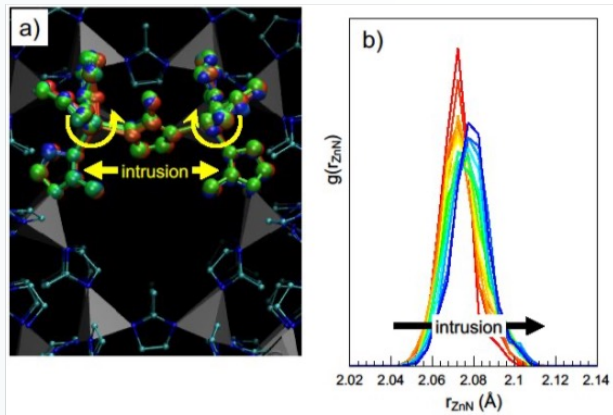
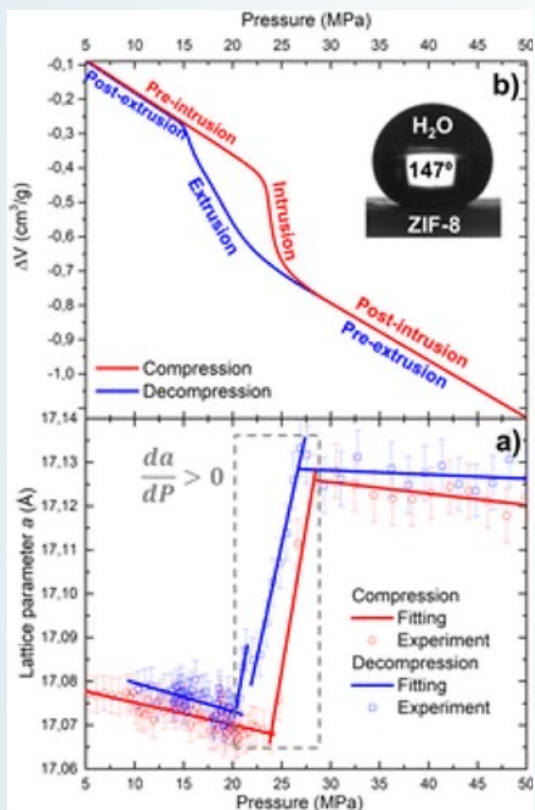
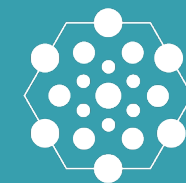


Tortora et al. *Nano Lett.* 2021, 21, 7, 2848–2853

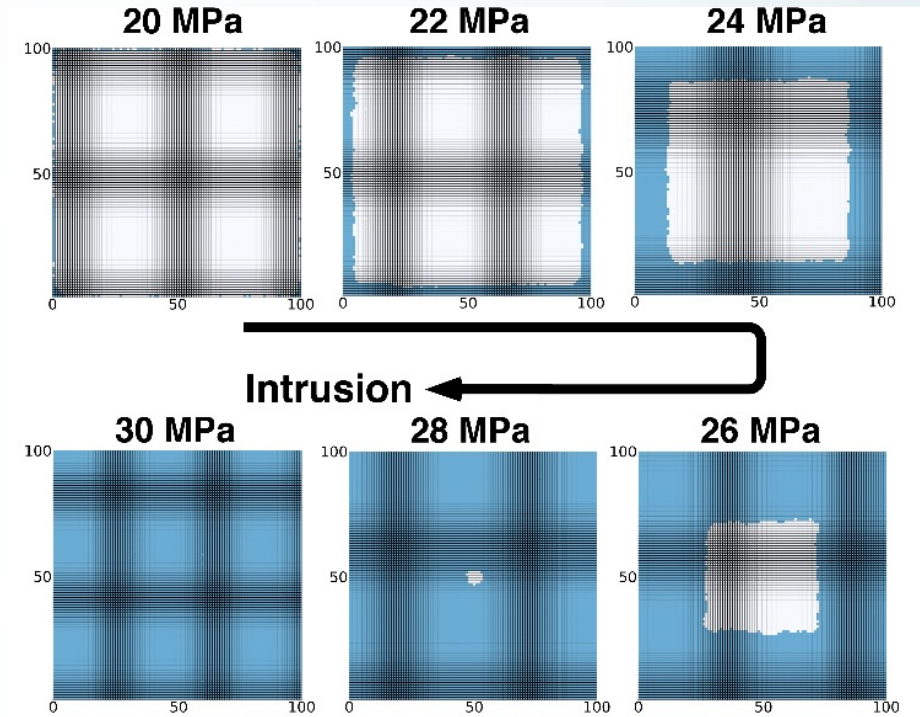
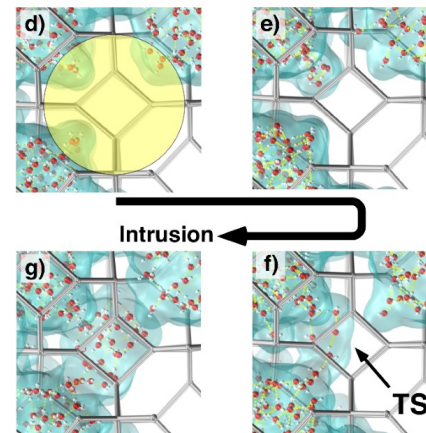
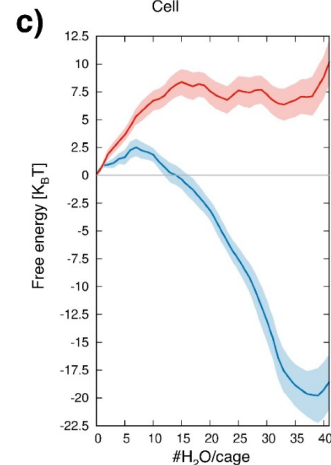
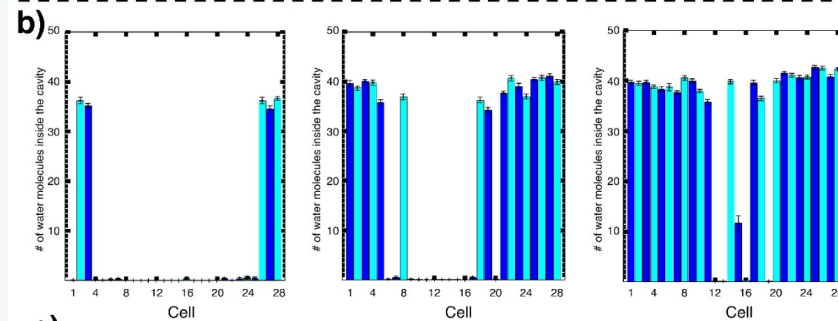
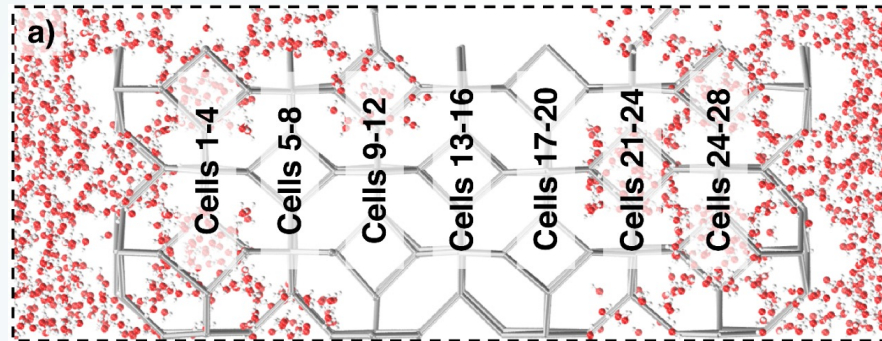
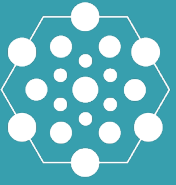


Bushuev, Y. G. et al. *Nano Lett.* 2022, 22(6), 2164-2169.

Strain Analysis of ZIF-8 Upon Intrusion

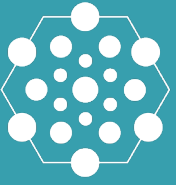


Evidence of Cage-by-Cage Bridging via RMD simulation



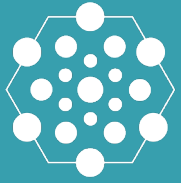
Amayuelas et al, *Nano Lett.*,
2023, Accepted

Conclusions and Future Direction



- We reveal intrusion via cage-by-cage movement from the exterior to interior pores
- "Bridging", the formation of a hydrogen bond network across pore windows, lowers the free-energy barrier until a critical threshold network is created, leading to cascade intrusion into the pore.
- This explains the presence of strain in the ZIF-8 lattice during the intrusion process, which dissipates once all cages are filled
- The pore interconnectivity is therefore a key design feature of a candidate material for Int/Ext-based devices.

Fellow Authors and Special Thanks



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Thanks for your attention!



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