M. Tortora, A. Le Donne, A. R. Lowe, M. Chorążewski, J. B. Leão, G. V. Jensen, M. Bleuel, A. Giacomello, C. M. Casciola, S. Meloni and Y. Grosu*

*andrea.ledonne@unife.it, University of Ferrara

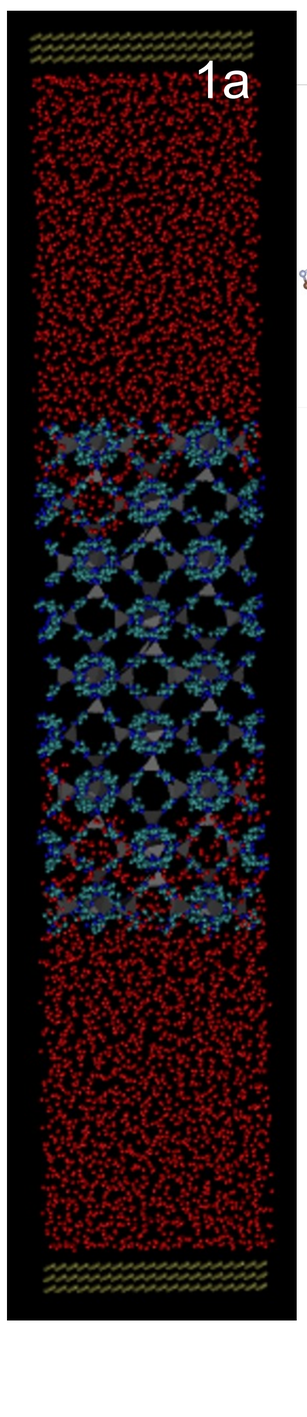
Università degli Studi di Ferrara

Giant Negative Compressibility by Liquid Intrusion into Superhydrophobic Flexible Nanoporous Frameworks

Introduction

Materials or systems demonstrating negative linear compressibility (NLC), whose size increases (decreases) in at least one of their dimensions upon compression (decompression) are very rare. NLC can be achieved using an auxetics and applying non-isotropic stresses, where the negative response is associated either with a porous auxetic geometry[1] or with elastic properties of the system[2] and can be predicted by computational methods. However, more recently, it has been shown that NLC can result also from the application of hydrostatic pressure to suitably designed negative Poisson's ratio materials.[3] Here, we show that one can achieve exceptional negative compressibility by nonwetting liquid intrusion into flexible porous media like ZIF-8, which present a final negative compressibility coefficients of ~10 3 TPa⁻.[4]

Results



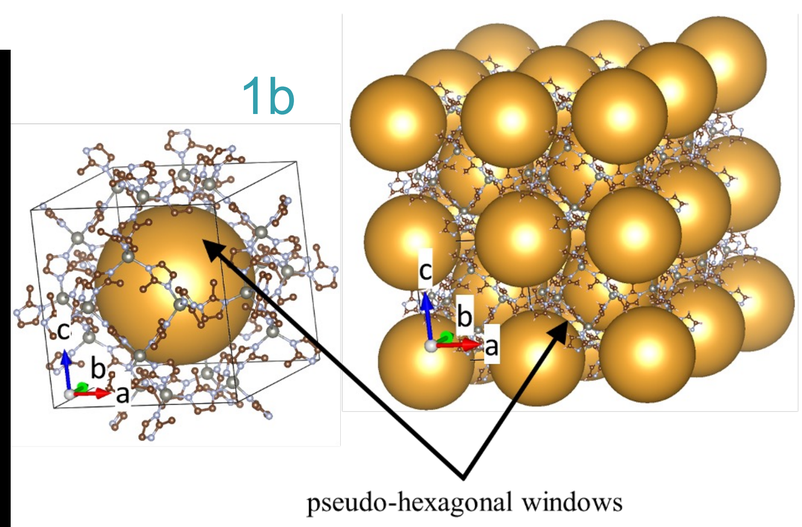


Figure 1a: Snapshot of the computational sample at a specific level of filling. Figure 1b: Unit cell (left) and crystalline structure of ZIF-8 (right). The large sphere at the center of the unit cell highlights the cavity that get filled by water during intrusion. The connection between different cavities occurs via the pseudo-hexagonal windows.

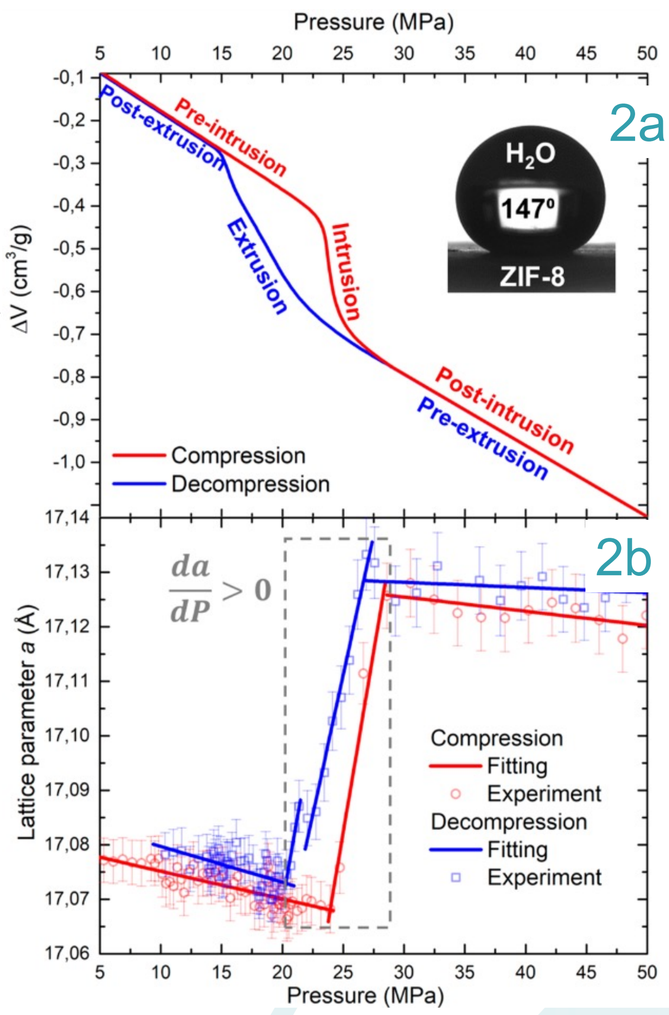


Figure 2a: Experimenta evolution of lattice parameter *a* with pressure.

Figure 2b: Experimenta PV-isotherm and contact angle.

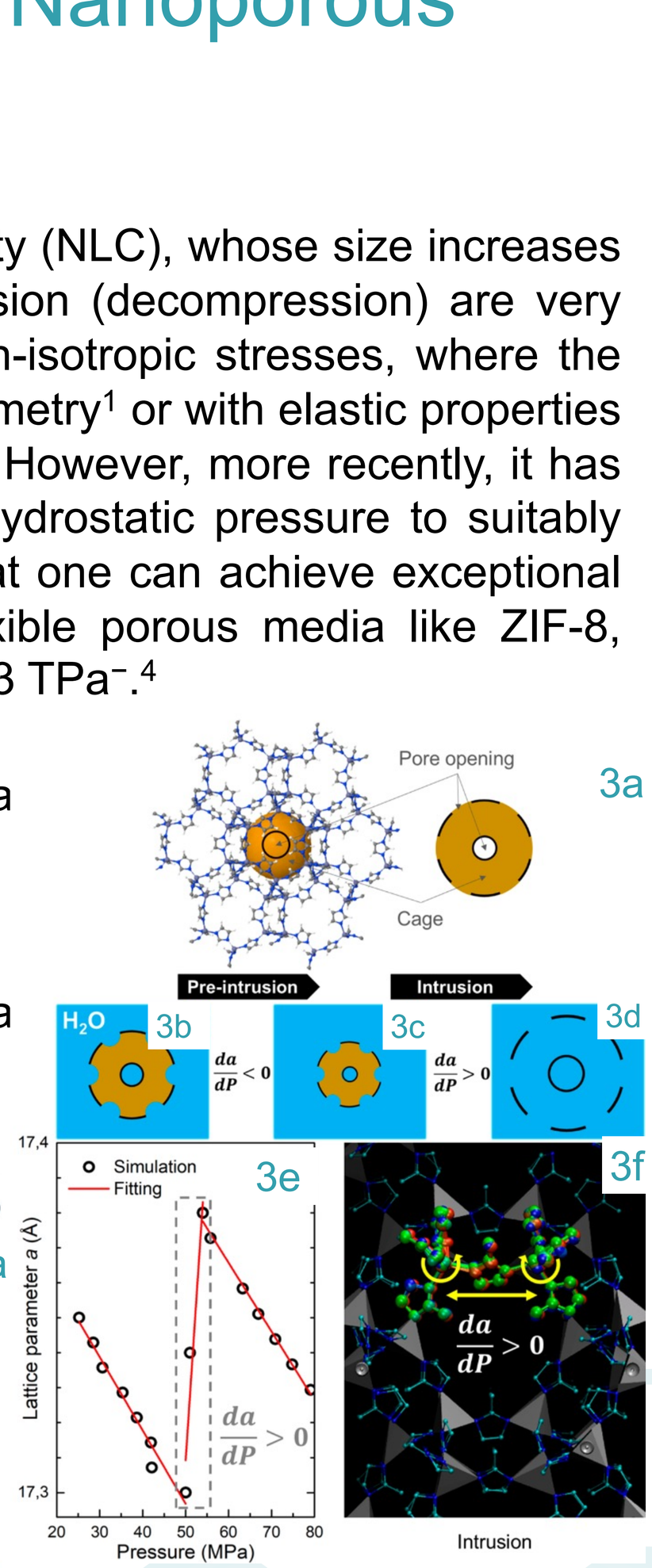


Figure 3a-d: Topological model of cavity of ZIF-8; schemes of framework response to compression before and during water intrusion, respectively. Figure 3e: Theoretical evolution of lattice parameter *a* with pressure; Figure 3f: Evolution of two connected ZnIm4 tetrahedra.

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