Energetic applications of Hydrophobic Nanopores: HPC and *in silico* design

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High Performance Computing and state-of-the art atomistic simulations can be used in order to reliably characterize the nanoscale wetting behavior of various classes of hydrophobic nanoporous materials that show great promise as novel, cheap and green methods of dissipating and storing mechanical energy [1-2]. Efficient, high density, energy storage in particular is going to be a topic of increasing popularity, especially due to the increasing challenges associated with the responsible use of energy in the upcoming future.

Most energetic applications of hydrophobic nanoporous materials are based on the possibility to build devices in which the porous materials is confined within a sealed container with a moving wall acting as a piston [3-4]. By applying a force on the moving wall it is possibile to raise the liquid pressure and have liquid (typically water) intrude within the dry pores of the material. Releasing the pressure it is then possible to revert to the initial conditions by triggering the extrusion of water from the pores, as implied by the hydrophobicity of the material. By cycling the pressure, mechanical energy can thus be converted into internal energy of the system (i.e. as surface tension) and then again into mechanical energy. Such devices can be extremely useful for all technological applications in which there is a necessity to efficiently and dissipate vibrations over a wide range of frequency, or to store and release mechanical energy with high energy density.

By deploying advanced Molecular Dynamics simulations, allowing for precise free-energy calculations, we have been successful in characterizing the thermally activated character of the pore wetting and drying processes [1-2]. In particular, atomistic simulations are among the few tools able to characterize the phenomenology of a single nanopore, in contrast with the inherently global view of more traditional intrusion-extrusion experiments.

A major achievement of our molecular simulations was to unravel the way in which the size of the pores drastically changes their behavior. Larger (D=2-3 nm) pores show an hysteretical behavior with radically different intrusion and extrusion pressures, thus allowing for the efficient dissipation of mechanical energy, while smaller pores (D~1.5 nm) are able to store mechanical energy and release it at a later stage with a ~1 efficiency. These findings, along with quantitative predictions on the energy storage and dissipation performances of such devices, are consistent with experimental observations on various classes of hydrophobic materials [1,3]

Molecular modeling of these materials, was only made possible by the availability of the vast computational resources provided by PRACE Grants (SLIP,MDGate @CINECA FERMI/MARCONI, and presently, as PI, the VaPore grant @GENCI Joliot-Curie). Tier-0 resources are indeed needed in order to simulate hundreds of replicas of our porous system on thousands of cores, allowing us to obtain precise insight over the thermodynamics and free-energetics of the wetting and drying processes.

1. Tinti et al. **PNAS** 114, (2017)
2. Tinti et al. **EPJ-E** 41, (2018)
3. Eroshenko et al. **JACS** 123 (2001)
4. Guillemot et al. **PNAS** 109, (2012)