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Molecular mechanisms and kinetics of water intrusion/extrusion into/from hydrophobic microporous nano-objects

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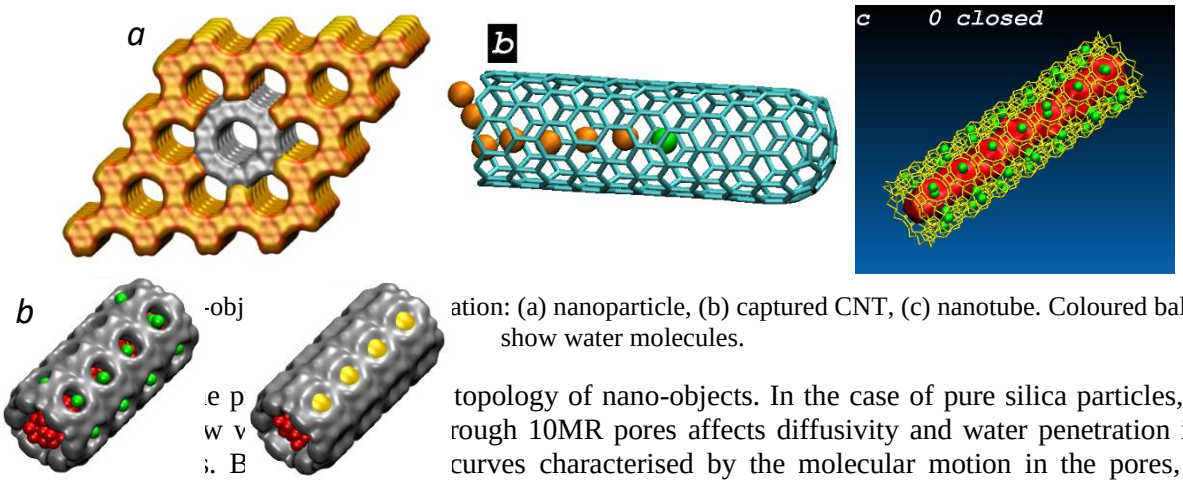
Establishing the molecular mechanisms of wetting and drying of hydrophobic porous materials is a general problem for science and technology within the subcategories of the theory of liquids, chromatography, and nanofluidics [1]. Microporosity plays a crucial role in the vital functions of living organisms.

We present results from molecular dynamics simulations of water intrusion/extrusion into/from nano-objects immersed in water, presented in Fig. 1: pure silica nanoparticles, carbon nanotubes, and nanotubes tailored from the ITT-type zeolitic framework, which has 18MR straight channels interconnected by 10MR lateral pores.



-obj ation: (a) nanoparticle, (b) captured CNT, (c) nanotube. Coloured balls show water molecules.

e p topology of nano-objects. In the case of pure silica particles, we w v rough 10MR pores affects diffusivity and water penetration into ;. B curves characterised by the molecular motion in the pores, we concluded that water in lateral pores stabilises water clusters in channels and promotes wetting of the nano-objects. Altering carbon-water interactions, we varied the preferential direction of molecular diffusion inside CNT and even CNT diffusion in water. Fast water expulsion from nanotubes with high hydrophobicity can be used as a nano-engine. Before complete water expulsion from nanoparticle channels, the number of molecules in the pores drastically decreases, destabilising water clusters. The metastable clusters lose connectivity, and molecules move fast to the channel's mouths. The process resembles the breaking of an over-stressed spring (Fig. 2).

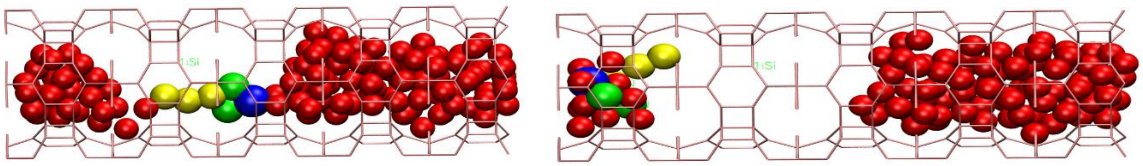


Figure 2: Molecular diffusion before water extrusion from 18MR channel. A time step for snapshots is 40 ps.

Demonstrated herein is that the diffusivity of water molecules in microporous objects is tightly connected with hydrophobicity and can be controlled by secondary porosity. This effect can be exploited to produce new materials for practical applications.

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References

[1] Y. G. Bushuev, M. A. Chorążewski, Y. Grosu, S. Meloni: *Subnanometer Topological Tuning of the Liquid Intrusion–Extrusion characteristics of Hydrophobic Micropores*. Nano Lett. **(in press)**, 10.1021/acs.nanolett.1c02140, (2022).