

Pore Morphology Determines Spontaneous Liquid Extrusion from Nanopores

Matteo Amabili,[†] Yaroslav Grosu,[‡] Alberto Giacomello,^{*,†} Simone Meloni,^{*,†} Abdelali Zaki,[‡] Francisco Bonilla,[‡] Abdessamad Faik,[‡] and Carlo Massimo Casciola[†]

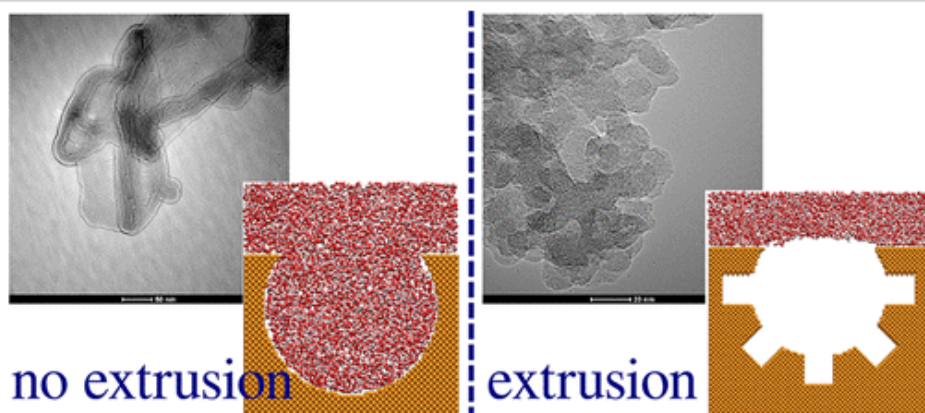
[†]Dipartimento di Ingegneria Meccanica e Aerospaziale, Sapienza Università di Roma, 00184 Rome, Italy

[‡]CIC Energigane, Albert Einstein 48, Miñano (Álava) 01510, Spain

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Abstract



In this contribution we explore by means of experiments, theory, and molecular dynamics the effect of pore morphology on the spontaneous extrusion of nonwetting liquids from nanopores. Understanding and controlling this phenomenon is central for manipulating nanoconfined liquids, *e.g.*, in nanofluidic applications, drug delivery, and oil extraction. Qualitatively different extrusion behaviors were observed in high-pressure water intrusion–extrusion experiments on porous materials with similar nominal diameter and hydrophobicity: macroscopic capillary models and molecular dynamics simulations revealed that the very presence or absence of extrusion is connected to the internal morphology of the pores and, in particular, to the presence of small-scale roughness or pore interconnections. Additional experiments with mercury confirmed that this mechanism is generic for nonwetting liquids and is rooted in the pore topology. The present results suggest a rational way to engineer heterogeneous systems for energy and nanofluidic applications in which the extrusion behavior can be controlled *via* the pore morphology.