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Confinement and hydrophilicity effects on geologically relevant fluids in silica nanopores

James Moraes de Almeida and Caetano Rodrigues Miranda
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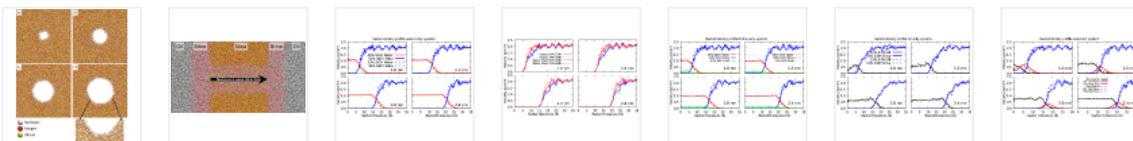
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ABSTRACT

Under extreme conditions, such as harsh thermodynamical environment and spatial confinement, fluids can reveal unique properties. In this work, we investigate the effects on the interfacial and transport properties of fluids confined in nanopores that are due to the spatial confinement, surface hydrophilicity, and fluid composition. We perform fully atomistic molecular dynamics of water, brine, oil, and combinations thereof, confined within amorphous silica nanopores with the radius ranging from 1.0 to 2.4 nm. We have also studied the oil infiltration on nanopores previously filled with water or brine, mimicking the natural processes when the oil is geologically formed and infiltrates a porous media. We observe that an adsorbed water/brine layer remains on the surface of the nanopores after the oil infiltration, altering the interaction of the oil with the confining surface and leading to changes of their interfacial tensions and viscosities. The presence of the ions in the brine thickens the adsorbed water layer, preventing the oil from infiltrating the nanopores with 1.0 nm radius. Thus, we have observed a limit on the pore size for oil infiltration for brine-filled pores.

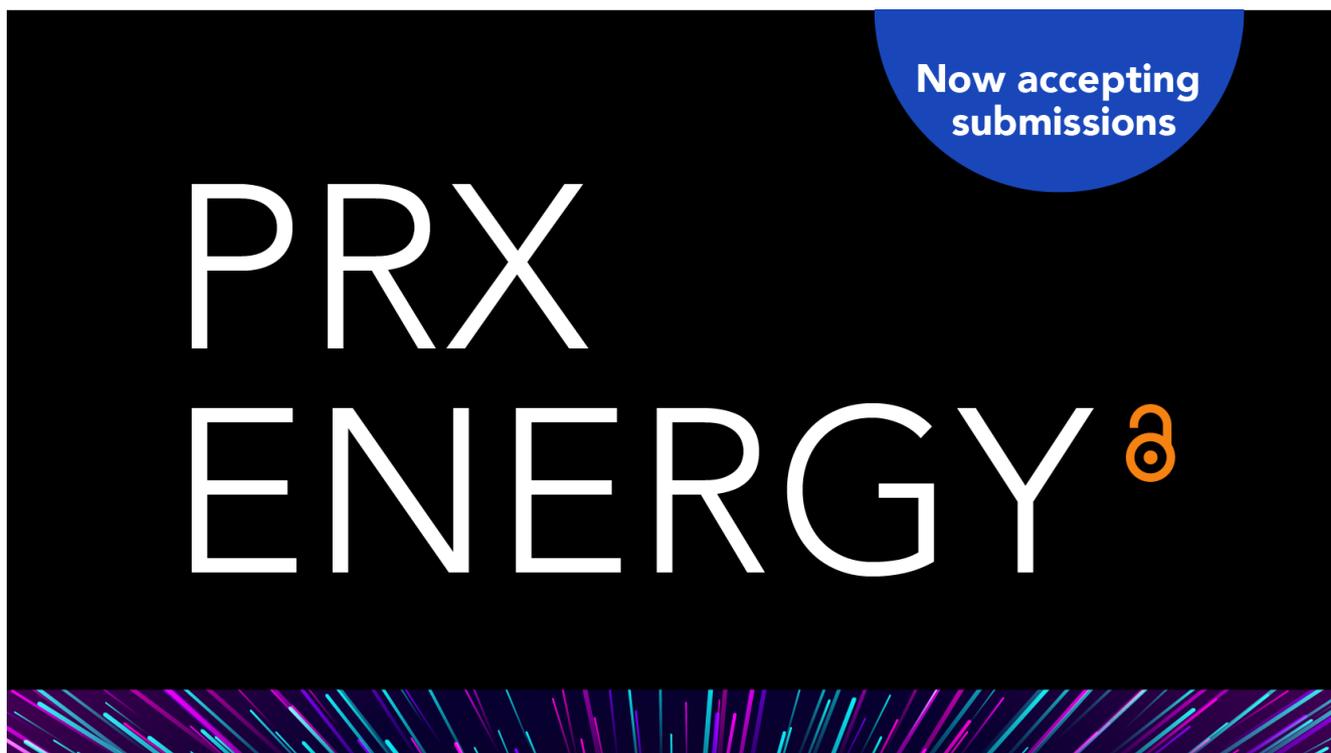


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