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Molecular Modeling of the Structure and Dynamics of Nanoconfined Fluids

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Understanding the structure and dynamics of fluids at nanoconfined interfaces is essential for continued progress in subsurface energy and environmental applications, and industrial applications such as catalysis, adsorption, and separations. Nanoscale structural, spectroscopic, and transport properties are readily obtained from molecular dynamics (MD) simulation, allowing the effects of fluid chemistry, pore surfaces, and pore size to be explored. Results will be presented for recent MD studies of nanopores comprised of amorphous silica and other materials, as well as a new force field for simulating bulk silica phases and silica-water interfaces. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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References

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