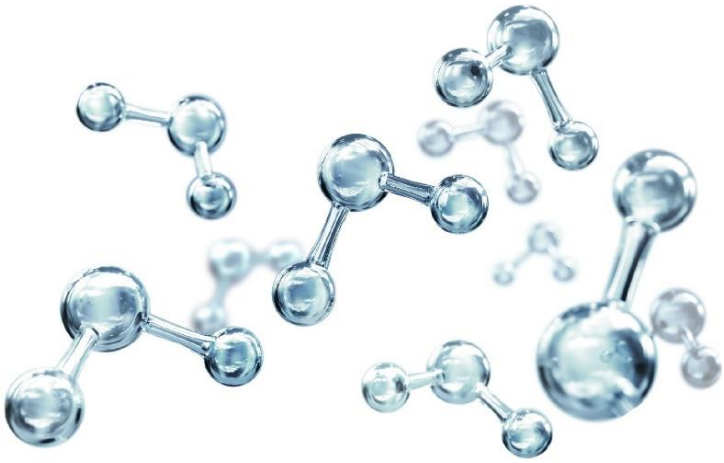
Seminar

CMWS Centre for Molecular Water Science

16th of October 2025
16:00 h (CEST)

Zoom Virtual Meeting:

https://tuhh.zoom.us/j/82631283465
Meeting-ID: 826 3128 3465
Password: 978444



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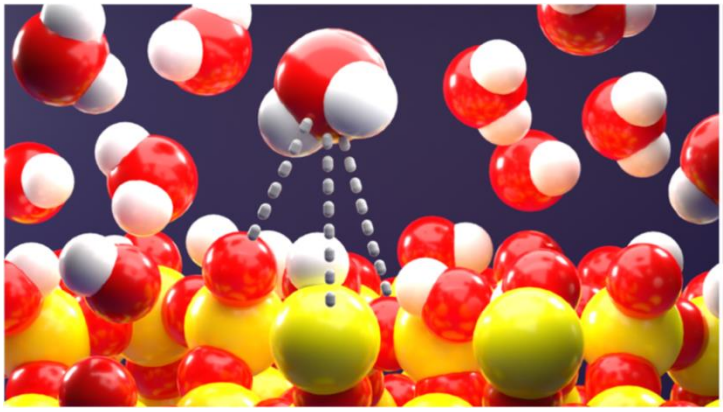
Confinement Effects on the Structure and Dynamics of Fluids from Molecular Simulation



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. 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 MD studies of nanopores comprised of amorphous silica and other materials, including a new force field (silica-DDEC) for simulating bulk silica phases and silica-fluid interfaces derived from density functional theory (DFT).[1] Subsequent efforts developing DFT-optimized parameters for silica-fluid interactions show significant differences in nanoconfined fluid properties for CO_2 and water compared to standard mixing rule approaches.[2-3] SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

[1] Senanayake, H. S.; Wimalasiri, P. N.; Godahewa, S. M.; Thompson, W. H.; Greathouse, J. A., Ab Initio-Derived Force Field for Amorphous Silica Interfaces for Use in Molecular Dynamics Simulations. *J. Phys. Chem. C* **2023**, *127*, 16567. https://dx.doi.org/10.1021/acs.jpcc.3c02270

[2] Godahewa, S. M.; Jayawardena, T.; Thompson, W. H.; Greathouse, J. A., Accurate Force Field for Carbon Dioxide-Silica Interactions Based on Density Functional Theory. *J. Phys. Chem. B* **2025**, *129*, 1122. https://dx.doi.org/10.1021/acs.jpcb.4c07413

[3] Jayawardena, T.; Godahewa, S. M.; Thompson, W. H.; Greathouse, J. A., Beyond Force Field Mixing Rules to Model Silica-Water Interfaces. *J. Phys. Chem. C* **2025**, *129*, 13394. https://dx.doi.org/10.1021/acs.jpcc.5c02442