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Extending equilibrium thermodynamics to include fluid-surface interaction for nanonconfined fluids

Monday, 31 May 2021 18:45 (15 minutes)

For nanoconfined fluids, equilibrium properties such as adsorption, density, and surface diffusion are dependent on the layered structure of the fluid near the surface. This layered structure is also relevant to describe transport as the noncontinuum effect, such as slip velocity, depends on the near-wall density. While molecular dynamics simulations quantify the layered density profile in nano-configurations, a systematic theoretical development to calculate equilibrium properties remains challenging. We consider a grand canonical ensemble and include fluid-surface interaction exclusively in the configurational integral. Using Lennard-Jones type interaction between the fluid and surface in the configurational integral, an approximation to the grand partition function for confined fluid is derived. Theoretically obtained density profiles are compared with grand canonical Monte Carlo simulations. While the focus of the present work is the density of the fluid, other static equilibrium properties and transport related quantities such as correction to slip can be derived using the surface-interaction corrected partition function.

Time Block Preference

Time Block C (18:00-21:00 CET)

References

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