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Full time and temperature scaling for nanoconfined fluids

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The behavior of fluids is strongly modified by spatial restrictions to the motion of the component particles and the particular interactions between the fluid and the confining walls. Such modification is particularly important for nanoconfined fluids where the pore diameter is $< 40s$ where s is the particle diameter. In nanoconfined systems, the distribution of particles gives rise to new wettability and layering phenomena in the vicinity of the pore wall, resulting in spatially dependent diffusion, which diverges strongly from that of the bulk behavior. The computation of the diffusion coefficient in these inhomogeneous fluids is an important topic in the study of both chemical and biophysical processes involved in nanoconfinement (examples) [cite]. The standard relation between the mean square displacement (MSD) and time is no longer valid. This is due to strong fluctuations in the fluid involving the forces present that have a range comparable to the system size. In this work we explore the influence of the particle wall interaction on the diffusive behavior of the fluid. In order to address this problem we use a combination of Virtual Layer Molecular Dynamics (VLMD) and the analytical solution for the MSD through a Langevin model for the inhomogeneous case. VLMD is a brand of Molecular Dynamics where the properties of the fluid are determined within artificially partitioned sections parallel to the fluid-wall interface, considering between them, absorbent boundary conditions. Layer properties are determined, and fed to the Langevin model, which is then solved.

Biography

Floralba Lopez has completed her MSc in Physics from Instituto Venezolano de Investigaciones Científicas (IVIC). She is a graduate student at the Faculty of Science, Universidad de Los Andes, Mérida – Venezuela.

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