Dynamical Behavior of Propane Under Nano-Confinement: Neutron Scattering Studies

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Molecular motion of carbon-bearing fluids in confined geometries, especially at extreme conditions of temperature and pressure, is an important area of research as it helps in the understanding of fluid-rock interactions in the terrestrial environment. An important tool in studying molecular motion in confinement is neutron scattering. This is because the energy and wavelength of cold and thermal neutrons are in the same range as that of the motions and spatial structure respectively of molecules confined in porous materials. We have used this technique to study the stochastic and vibrational dynamics of propane confined in silica materials, serving as proxies for silica rich rocks, at temperatures and pressures relevant to terrestrial environments. Interaction of the propane molecules with the pore wall is found to play an important role in the stochastic motion of propane confined in silica aerogel. It was found that at low pressures propane molecules get strongly adsorbed at the pore walls and are therefore mostly immobile whereas at high pressures, more propane molecules are available near the pore centers and they get involved in the dynamics thereby enhancing the diffusion coefficient. Further, presence of CO_2 was also found to enhance the diffusivity of propane in silica aerogel. Confinement of propane in MCM-41-S was found to affect its vibrational behavior. The low energy vibrational spectra of confined propane exhibited glassy behavior. This behavior was further found to be pressure dependent. MD modeling has been done to provide molecular-level insight into the behavior of propane in nanopores.