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Molecular dynamic simulations for studying methane/water systems: Diffusion and structure

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Molecular dynamic simulations have been performed to investigate thermodynamic and structural properties of methane/water system at two different conditions away from hydrate formation and threshold it. One of the main motivations to study the methane/water system is related to formation of gas hydrates. Gas hydrates are crystalline inclusion compounds consisting of water molecules forming cages via a hydrogen-bonding network and enclosing small guest molecules such as methane, ethane, CO₂, etc. Methane gas hydrates studies are more noteworthy because of future energy source and the problems they pose to the petroleum industry during the production and transportation. The results that compare the two conditions have been discussed in terms of the surface tension, mean square displacement (MSD), diffusion coefficient, radial distribution function and thermodynamic functions. Investigation over a timescale of 500 ps demonstrated that the thermodynamic functions at 275 K (at hydrate formation threshold) are smaller than that of at 298 K, implying that the hydrate formation threshold is more stable. An increase in the system pressure and temperature leads to a decrease in surface tension because of the decrease in the intermolecular attractive forces. The comparison of oxygen-oxygen, carbon-carbon and carbon-oxygen radial distribution functions at temperatures of 275 and 298 K has been indicated that all distribution peaks decrease due to increasing the temperature demonstrating that the system become more stable at threshold of hydrate formation. MSD and self-diffusion coefficient of methane molecules are sensitive to the temperature and pressure of system.

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