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Insight on the stability of gas hydrate in montmorillonite slits by molecular dynamics simulations

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The extent of interactions between clay surfaces and water molecules and their impact on hydrate stability in clay reservoirs have been a source of debate. This uncertainty arises from the inherent challenges associated with the nanoscale temporal and spatial detection of bound water molecule distribution characteristics. This study employs molecular dynamics simulations to investigate the stability of methane hydrates in montmorillonite slits at various temperatures, focusing on the surface influence scale, bound water molecule distribution characteristics, and binding strength. The results show that hydrates in close proximity to the clay surface exhibit lower stability and are more prone to decomposition. The hydrophilic nature of the surface leads to water molecule aggregation at the interface, driving methane molecules away during decomposition. Additionally, compared to the charged tetrahedral layer surface of montmorillonite, the quasi-liquid layer on the neutral tetrahedral layer surface is thinner, with semicage structures persisting within the vacancies of the Si-O rings. The analysis suggests that variations in the range of surface influence and binding strength can be primarily attributed to intermolecular Coulomb interactions and charge redistribution at the interface. These research findings offer valuable molecular insights into the microscopic characteristics and behavior of hydrates within clay slits.

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