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Molecular-Dynamics Study of H_2-C_3H_8-Hydrate Dissociation: Non-Equilibrium Analysis

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Abstract : Hydrogen is looked upon as the next-generation clean-energy carrier; the search for an efficient material and method for storing hydrogen has been, and is, pursued relentlessly. Clathrate hydrates are inclusion compounds wherein guest gas molecules like hydrogen are trapped in a host water-lattice framework. These types of materials can be categorised as potentially attractive hosting environments for physical hydrogen storage (i.e., no chemical reaction upon storage). Non-equilibrium molecular dynamics (NEMD) simulations have been performed to investigate thermal-driven break-up of propane-hydrate interfaces with liquid water at 270-300 K, with the propane hydrate containing either one or no hydrogen molecule in each of its small cavities. In addition, two types of hydrate-surface water-lattice molecular termination were adopted, at the hydrate edge with water: a 001-direct surface cleavage and one with completed cages. The geometric hydrate-ice-liquid distinction criteria of Báez and Clancy were employed to distinguish between the hydrate, ice lattices, and liquid-phase. Consequently, the melting temperatures of interface were estimated, and dissociation rates were observed to be strongly dependent on temperature, with higher dissociation rates at larger over-temperatures vis-à-vis melting. The different hydrate-edge terminations for the hydrate-water interface led to statistically-significant differences in the observed melting point and dissociation profile: it was found that the clathrate with the planar interface melts at around 280 K, whilst the melting temperature of the cage-completed interface was determined to be circa 270 K.

Keywords : hydrogen storage, clathrate hydrate, molecular dynamics, thermal dissociation
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