Mechanism and Thermal Conductivity Variation in Physisorption: A Molecular Dynamic Study

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論　文　審　査　の　結　果　の　要　旨

The physical adsorption of gases has been widely applied in gas storage, thermal energy utilization, and environmental purification. A great deal of research works has been reported primarily on the synthesis and characterization of adsorbents, equilibrium uptake and adsorption kinetics from the perspectives of heat and mass transfer mechanisms. However, molecular scale adsorbate diffusion mechanism within adsorbents has not been understood completely.

Meanwhile, understanding the changes in thermodynamic and transport properties during adsorption is essential for optimizing thermal management in adsorbent-based systems. Thermal conductivity, a key transport property, plays a critical role in enhancing performance and energy density but presents notable challenges due to the complexities of phase transitions and variations in intermolecular interactions during adsorption. Contradictory hypotheses regarding thermal conductivity behavior within adsorption systems highlight the need for deeper investigation.

In the study, molecular dynamics simulations had been employed to elucidate the adsorption and diffusion behaviors of methane in its liquid state at low-temperature, gaseous state at low-temperature, and gaseous state at room-temperature in Cu-BTC. The main findings of the study are summarized below.

- Based on the energy distribution and dynamic trajectories of the adsorbed molecules, the author proposed a hypothesis that the adsorbed phase could be classified into four distinct types: bound molecules (oscillate around a specific region of the adsorbent), generally adsorbed molecules (within the range of interaction from the surface, and possess negative total energy), non-adsorbed molecules (within the range of interaction from the surface, but having positive total energy, and the ability to escape), and free molecules (beyond the range of interaction from the surface). To further support the hypothesis, the concepts of absolute adsorption and excess adsorption were implemented, where methane adsorption in MOF-5 was simulated and compared with existing experimental data. The results showed that using

energy distribution to evaluate absolute and excess adsorption had broader applicability.

- Detailed MD simulations were used to replicate methane adsorption in Cu-BTC and evaluated thermal conductivities under different pressures and temperatures. The results revealed significant variations in the thermal conductivities of both the adsorbent (Cu-BTC) and the adsorbed phase (methane).

In conclusion, the study provided insights into the adsorption behavior in molecular scale, and advanced the understanding of adsorption thermodynamics and transport properties. The main findings of the study offered valuable perspectives for the design of energy-efficient adsorption systems, and contributed greatly to the progress of interdisciplinary research field of adsorption science and thermal engineering. Therefore, the author of the thesis deserves to receive Doctor of Philosophy.