Characterization of Solid-like Adsorption of Hydrogen on Porous Materials Using BET Method: A Molecular Simulation Study

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Recently, solid-like adsorption of hydrogen on mesoporous silica material at 20 K has been experimentally observed, but the origin of high-density hydrogen adsorption is still in debate. In this work, GCMC simulations and BET analyses were carried out on for different metal-organic frameworks(MOFs) and a model homogeneous CNT pore (d = 10 nm) to elucidate the origin of solid-like hydrogen adsorption at low temperature. Molecular simulation snapshots were analyzed and compared with the BET area calculated from the adsorption isotherm to test the validity of consistency criteria from BET theory