

Structure analysis of clathrate hydrate for hydrogen storage using Monte Carlo simulation

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It is desirable to develop new materials that can store large amounts of hydrogen for portable electronics and moving vehicles. Clathrate hydrates of hydrogen have been proposed recently as hydrogen storage. According to recently reported method, the structure II (sII) hydrates of hydrogen and tetrahydrofuran can store about 4wt% of hydrogen at modest pressures. However, these double hydrates still don't have sufficient capacity to use commercial hydrogen storage. Therefore, theoretical simulation study is required to use clathrate hydrates for hydrogen storage. In this work, the structure of double hydrate is studied by Monte Carlo simulation in NPT ensemble. Lennard-Jones potential and Coulomb potential model are applied to simulate between molecules.