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单壁碳纳米管中甲烷吸附的分子模拟

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摘要 采用巨正则系统MonteCarlo方法研究了甲烷在单壁碳纳米管(Singlewallcarbonnanotube,SWNT)中于低温74.05K下的吸附等温线及吸附机理，发现在两个较小的孔径(1.225nm和1.632nm)下单壁碳纳米管中甲烷的吸附有着明显的微孔所独有的“填充效应”，而在2.04nm以上的孔的吸附中会出现毛细凝聚现象。通过模拟知道发生毛细凝聚的必要条件是孔内能至少容纳下两层粒子，此外还导出在恒定温度下毛细凝聚吸附量与SWNT孔径关系。本文还模拟了常温300K下甲烷在SWNT内的吸附，对比了2.04nm和4.077nm两种孔径的SWNT吸附甲烷的等温线，推荐在4.077nm孔中的适宜吸附存储压力为5.0～6.0MPa，吸附质量分数可达16%～19%.

关键词 甲烷 吸附 计算机模拟 蒙特卡罗模拟

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Molecular simulation on adsorption of methane in single wall carbon nanotubes

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Abstract By using grand canonical ensemble Monte Carlo method, machanism for the adsorption of methane in single wall carbon nanotubes(SWNTs) at 74.05 K has been investigated. It is found that the adsorption of methane in smaller SWNTs, whose diameters are 1.22nm and 1.632nm, exhibits "pore filling" behavior. In contrast, for the SWNTs of diameter larger than 2.04nm, capillary condesation takes place. Simulation shows that the required condition for the capillary condensation is that two layers of molecules can be accommodated in SWNTs. In addition, a relationship between the quantity of methane adsorbed and the diameter of SWNT for the capillary condensation is developed. A comparison of the isotherms for the SWNT diameters of 2. 04 nm and 4.077nm at ambient temperature, T=300 K, indicates that proper adsorption pressure range is 5.0～6.0 MPa. In this case, the weight fraction of adsorbate is about 16%～19%.

Key words METHANE ADSORPTION COMPUTERIZED SIMULATION MONTECARLO SIMULATIONS

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