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乙烷在单壁碳纳米管中的密度泛函理论研究

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摘要 Density functional theory (DFT) is used to calculate adsorption of ethane molecules in single walled carbon nanotubes. A compari-son of DFT calculations and grand canonical ensemble Monte Carlo (GCMC) simulations is made first and the two methods are in good agree-ment. Adsorption isotherms and structures of ethane molecules inside the tubes have been studied by DFT for the nanotubes of diameters 0.954,2.719 and 4.077 nm at 157 K and ambient temperature, 300 K. By using the grand potential, the positions of phase transitions are exactly lo-cated, and the effect of temperature and tube diameter on phase transitions and adsorption is discussed. We found that lowering temperature andincreasing the pore size of several nanometer is preferable for the ethane adsorption when temperature is in the range of 157 K-300 K and op-erating pressure reaches several MPa. Layering transitions and capillary condensations are observed at 157 K in two larger pore diameters,while these phase transitions disappear or the hysteres is loops become very narrow at 300 K.

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Ethane Adsorption in Single Walled Carbon Nanotube by Density Functional Theory

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Abstract Density functional theory (DFT) is used to calculate adsorption of ethane molecules in single walled carbon nanotubes. A compari-son of DFT calculations and grand canonical ensemble Monte Carlo (GCMC) simulations is made first and the two methods are in good agree-ment. Adsorption isotherms and structures of ethane molecules inside the tubes have been studied by DFT for the nanotubes of diameters 0.954,2.719 and 4.077 nm at 157 K and ambient temperature, 300 K. By using the grand potential, the positions of phase transitions are exactly lo-cated, and the effect of temperature and tube diameter on phase transitions and adsorption is discussed. We found that lowering temperature andincreasing the pore size of several nanometer is preferable for the ethane adsorption when temperature is in the range of 157 K-300 K and op-erating pressure reaches several MPa. Layering transitions and capillary condensations are observed at 157 K in two larger pore diameters,while these phase transitions disappear or the hysteres is loops become very narrow at 300 K.

Key words density functional theory; adsorption; ethane; single walled carbon nanotube

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