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研究论文

# 金属-有机骨架材料中甲烷吸附机理的密度泛函理论研究

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摘要 采用密度泛函理论研究了甲烷在MOF-5中的吸附位置、吸附构型和吸附能. 结果表明: 吸附位置主要有四种, $Zn_4O$簇为最佳吸附位, 其吸附能为17.38 kJ•mol$^{-1}$, 高于沸石中的甲烷吸附能. 从吸附能与MOF-5的结构关系分析得出: 在苯环中引入给电子基团, 有利于增强甲烷与MOFs的吸附作用; 引入含氧等极性官能团, 将增加甲烷吸附位, 有利于提高吸附储存量.

关键词 甲烷 金属-有机骨架材料 吸附 密度泛函理论

分类号

# A Density Functional Theory Study of Methane Adsorption Mechanism in a Metal-Organic Framework

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**Abstract** The density functional theory was used to study the adsorption sites, conformation and the adsorption energies of methane in MOF-5. The results show that there are four adsorption sites, and the $Zn_4O$ clusters are the preferential adsorption sites, for which the adsorption energy is 17.38 kJ•mol$^{-1}$, larger than that in zeolites. This work shows that the adsorption energy around the aromatic rings can be increased by introducing electron-donor functional groups. In addition, the introduction of polar functional groups such as O containing groups to the organic linkers can introduce additional adsorption sites that increase methane adsorption capacity.

**Key words** methane metal-organic framework adsorption density functional theory

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