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论文

分子动力学模拟1-丁烯和正丁烷在MCM-22分子筛中的扩散行为

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摘要:

应用分子动力学方法研究了1-丁烯和正丁烷在MCM-22型分子筛(ITQ-1)中的扩散行为. 得到了两种物质在ITQ-1分子筛两个独立孔道中的均方位移曲线、自扩散系数和扩散轨迹. 计算结果表明, 在温度为400 K时, 1-丁烯或正丁烷在十元环孔道中的扩散明显低于在超笼中的扩散, 吸附质在超笼的底部和顶部的扩散明显低于在超笼中心的扩散; 1-丁烯和正丁烷在ITQ-1分子筛的超笼中两者扩散速率较为相似, 而在十元环中, 两者的扩散速率差别较大.可以推测, 选择性催化主要发生在十元环中.

关键词: ITQ-1分子筛; 分子动力学模拟; 1-丁烯; 正丁烷

Molecular Dynamics Simulation for Diffusion of 1-Butene and n-Butane in MCM-22 Zeolite

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Abstract:

The molecular dynamics techniques were used to simulate the diffusion of 1-butene and n-butane in purely siliceous ITQ-1 zeolite. The mean square displacement(MSD) plots, diffusion trajectories, and diffusion coefficients of 1-butene and n-butane were obtained. The results show that the molecules of 1-butene and *n*-butane can diffuse in the different independence channel systems of ITQ-1 zeolite at 400 K; the diffusion capability of 1-butene is less than that of *n*-butane. The differences in diffusivity were observed between 1-butene and n-butane, especially in the sinusoidal 10 member ring system. Similar features in the diffusivity were observed in the supercages. The diffusion and migration of 1-butene and n-butane mainly occurred in supercage system. On the other hand, the diffusion of those adsorbates at the center of the supercage is easier than those at the upper and lower of the supercage. It indicated that the reaction of the skeletal isomerization happen in 10-MR channel systems.

Keywords: ITQ-1 zeolite; Molecular dynamics simulation; 1-Butene; *n*-Butane

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