A molecular dynamics investigation of template molecule in the zeolite channel

Angyang Yu

Liaoning University of Petroleum and Chemical technology, Fushun; 113001, China

Abstract

The location and diffusion properties of template molecules in the zeolite channel have been investigated based on molecular dynamics method. Simulation results show that template molecules can reside in the supercages and the sinusoidal channels of the zeolite with good stability. It has been found that template molecules can diffuse easier in the supercages than in the sinusoidal channels, which means that template molecules can desorpt from the supercages more easily. Since the template molecules are nearly still in the sinusoidal channels, we can conclude that the template molecules can bind strongly with the sinusoidal channels, with a high desorption temperature. Additionally, the decomposition of the template molecules has happened before desorption from the zeolite.

Keywords

Molecular dynamics; Template molecules; Zeolite; Desorption