



BERKELEY CATALYSIS CENTER

Distinguished Lecture Series

Monday April 24, 2006

775-B Tan Hall

10:00 a.m.-12:00 p.m.

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“Intracrystalline Diffusion Processes in 8-Ring Crystalline Microporous Materials: Window Size Effects”

ABSTRACT:

The diffusion of gases and hydrocarbons in porous materials is a subject of great practical importance in the chemical and petrochemical industry. Porous materials are widely utilized as adsorbents, membranes, and catalysts. The growing interest in porous solids is fueled by ever-expanding possibilities in synthesis routes that are leading to optimally designed materials with controlled structure and composition. For example, crystalline microporous materials that selectively control diffusion through 8-member ring window apertures are becoming particularly useful for an emerging class of adsorptive separations that rely on kinetics rather than equilibrium. Some of the challenges of kinetic separations are the synthesis of materials with precisely controlled window apertures and the proper characterization of diffusion over a wide range of time scales.

This presentation will highlight the use of some unique complementary techniques (e.g., frequency response and Pulsed Field Gradient NMR) for measuring intracrystalline diffusion in materials that have great potential for kinetic separations. It will be shown that pure silica 8-ring microporous materials are ideally suited for separating, for example, propylene from propane (CHA) and carbon dioxide from methane (DDR). These separations are of great practical importance and difficult to carry out conventionally. It will also be shown that the rates of diffusion in these cation-free materials can be advantageously modified by changes in framework composition. Thus, for example, the rates of diffusion can be increased by orders of magnitude when the CHA structure is prepared in aluminophosphate form instead of pure silica. Supported by X-ray data, such results are consistent with a slightly smaller window size in the later material. Finally, to demonstrate the generality of these framework composition effects, the rate of propylene diffusion in the LTA structure in aluminosilicate and in pure silica form will also be contrasted. The results will show again that an increase in window size is responsible for the greater diffusion in the aluminosilicate, notwithstanding the presence of extra-framework balancing cations.