New horizons for diffusion research in nanoporous materials: Experiments, Theory and Application.

Diffusion in zeolites – a never-ending story?

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Economic motivation of our activities in technical application
ZEOLITE SYNTHESIS (J. Caro)

Non-Equilibrium Techniques (transport diffusion)
- Coherent QENS (H. Jobic)
- Interference Microscopy (J. Kärger)
- IR Microscopy (J. Kärger)
- Single-Crystal Permeation (D.B. Shah)
- ZLC (S. Brandani)
- FR (A. Jentys, J. Lercher)
- Uptake/Release (R. Staudt)

Equilibrium Techniques (self-diffusion)
- Incoherent QENS (H. Jobic)
- (MAS) PFG NMR (P. Galvosas, J. Kärger)
- Tracer IR Microscopy (J. Kärger)
- Tracer Single-Crystal Permeation (D.B. Shah)
- Tracer ZLC (S. Brandani)
- Tracer Exchange (R. Staudt)

Observation range:
- nanometers
- micrometers
- individual crystals
- crystal assemblage
What do we measure?

Interference Microscopy (IFM)

\[ j = - D_{(T)} \text{grad } c \]

transport diffusion

Pulsed Field Gradient (PFG) NMR

\[ \langle r^2(t) \rangle = 2Dt \]

self-diffusion
Intracrystalline Diffusion

Comparison of the PFG NMR results with the results of MC simulations

n-Butane / Silicalite-1

two sets of measurement with different samples

\[ p_y = 1 \quad p_x = 0.32 \]
\[ p_z = 0.067 \quad [1] \]

\[ (E_b - E_d) = 21.5 \text{ kJ/mol} \]
\[ N = 3000 \times 1\text{nm} \]
Interference Microscopy (IFM): Influence of defects on the external crystal surface on the isobutane uptake into MFI-type zeolite

The non-etched sample (strong surface barriers)

Faster desorption in the middle part of the crystals than near crystal edges: desorption through the crack surface

Faster desorption in the crystal part with the crack

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J. Kärger: Diffusion in zeolites – a never-ending story?
The etched sample (mild surface barriers)

- Desorption through the crack surface

(i) Both the diffusivity and permeability of transport barriers determine the rate of desorption
(ii) Faster desorption in the crystal part with the crack

The etched sample (mild surface barriers)
Medical diagnosis has attained such a high level that there scarcely exist any really healthy people.
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• Diffusion in zeolites – a never-ending story?
  Prof. J. Kärger, Universität Leipzig

• Diffusion studies by QENS – measurements approaching the „ideal“ situation
  Dr. H. Jobic, Institut de Recherche sur la Catalyse, Villeurbanne, France

• Correlating molecular modelling and experimental diffusivities
  Prof. D. Theodorou, National Technical University of Athens, Greece

• Ideal vs. Real zeolite structure: options to discriminate
  Prof. J. Caro, Universität Hannover

• Studying „macroscopic“ aspects of diffusion
  Prof. S. Brandani, University College London

• From diffusion research to industrial application
  Prof. D. Ruthven, University of Maine, Orono, Maine, USA

• Mass transfer coefficients determined from break-through experiments
  Dr. J. Oppermann, Linde AG, Höllriegelskreuth