

Ústav fyzikální chemie J. Heyrovského, v.v.i.
Akademie věd České republiky

zve všechny zájemce na ústavní seminář,
na kterém promluví

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na téma

**Sorption, transport, and catalytic
transformations of hydrocarbons in
microporous materials**

Seminář se koná
v pondělí 15. října 2012 od 14:00 hodin
v Brdičkově posluchárně ústavu
v Praze 8, Dolejškova 3.

Těšíme se na Vaši účast. Hosté jsou vítáni.



**Sorption, transport, and catalytic transformations of
hydrocarbons in microporous materials**

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Microporous materials are a key element of catalysts in hydrocarbon catalysis utilizing both the catalytic activity of Brønsted and Lewis acid sites as well as the stabilization of the confines to catalyze transformations. The confines allow, thus, on the one side catalyzing hydrocarbon reactions more efficiently, but on the other side limit also the transport of reactants to these sites. Similarly, the spacing of acid sites in the pores strongly influence strength and catalytic activity in hydrocarbon transformations. Chances and limitations of the materials triggered a remarkable activity in synthetic and post-synthetic approaches to create new materials structured from the nano- to the mesoscopic level, such as hierarchical zeolites.

The lecture will describe efforts to manipulate and tailor three of the elementary steps, diffusion into and in pores of microporous materials, the adsorption at acid sites and the acid catalyzed conversion at these sites. With respect to transport into microporous materials, it will be shown that modifying the outer zeolite surface by overlayers enhances the probability of colliding molecules entering pores by increasing the sticking coefficient and reducing so surface barriers for diffusion. This effect is limited to small crystallites and will be masked by pore controlled diffusion in larger materials. Adsorbed in pores, the largest contribution to bonding is physisorption. Narrower pores over-proportionally reduce the entropy by limiting the configurational space. While aliphatic hydrocarbons have no problem approaching acid sites in zeolites, access is always challenged for aromatic molecules. Kinetically controlled catalytic conversions show clearly that the local stabilization of the carbocation defines the overall chemistry. Thus, the distribution of acid sites exerts an important influence on the acid catalyzed transformations. The three steps will be discussed using the alkane and alkene cracking as well as alkylation as examples. The potential and limitations for material synthesis to develop new catalysts will be discussed.

