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

---

zve všechny zájemce na ústavní seminář,
na kterém promluví

Tomáš Bucko

Comenius University, Bratislava, Slovakia

na téma

Molecular dynamics simulations of alkane conversions catalyzed by acidic zeolites

Seminář se koná
v úterý 11. prosince 2012 od 14:30 hodin
v Brdičkově posluchárně ústavu
v Praze 8, Dolejškova 3.

Těšíme se na Vaši účast. Hosté jsou vítáni.

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

Molecular dynamics simulations of alkane conversions catalyzed by acidic zeolites

Tomáš Bucko

Comenius University, Bratislava, Slovakia

Transition state theory provides the theoretical background to study reaction kinetics and its harmonic approximation (h-TST) can be considered as the current standard in ab-initio simulations. Despite its success in molecular chemistry, the harmonic transition state theory has several serious drawbacks. Often, however, the h-TST is used in simulations routinely and without judicious considerations. Although the methods designed to treat dynamical effects accurately have been developed, they are not widely used by ab-initio practitioners. Perhaps the most important reason that hinders propagation of these methods is that they are extremely demanding in terms of computational power. In my presentation, I will discuss a class of chemical reactions for which h-TST fails. It will be shown that accurate treatment of entropy is necessary not only for understanding of reaction kinetics but even for identification of correct reaction mechanisms. Results will be demonstrated on a “real-world” example of alkane conversions catalyzed by acidic zeolites.