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VABILO NA PREGLOV KOLOKVIJ / INVITATION TO THE PREGL COLLOQUIUM

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Četrtek / Thursday, 7. 03. 2013, ob / at 13:00

Velika predavalnica Kemijskega inštituta / Lecture Hall at the National Institute of Chemistry; Hajdrihova 19, Ljubljana

Catalytic alkane activation and transformation

Abstract*:*
In the light of the rapidly changing nature of the raw material basis of energy carriers and the back integration of petrochemical processes new challenges arise to selectively activate and convert light alkanes. Such new approaches could emerge from the drastically improved understanding of the interaction of light alkanes with solid surfaces and the surface chemistry induced by these interactions.
The lecture will illustrate how understanding the of the elementary steps involved in these elementary processes is a prerequisite to design and realize new generations of catalysts. Three examples are chosen, the bifunctional activation and dehydrogenation of alkanes in microporous materials, the oxidative dehydrogenation of ethane to ethane and the functionalization of methane. While the sorption and initial interaction of alkanes with the catalytically active surface is largely based on dispersion forces, the specific activation step depends subtly on the chemical and steric nature of the active site. It will be shown that bifunctional interactions help to drastically lower the energy barriers and enhance so catalytic activity. The activation process may involve ionic transition states in the case of strong Brønsted acid sites being present, as well as radical steps, when sites able forming radicals in a static and dynamic way are present. It will be discussed, how the active surface may interact with the initial products and what measures can be taken to protect the products. Chances and limitations of the potential reaction routes will be discussed.

Vljudno vabljeni! / Kindly invited!

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