chemisch physikalische gesellschaft

Gegründet im Jahre 1869 von H. Hlasiwetz, J. Loschmidt, J. Petzval und J. Stefan

Center for Computational Materials Science

EINLADUNG

zum Vortrag

von

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The Brønsted Acidity of Zeolites and the Activation of Hydrocarbons for Catalytic Conversion

am

Dienstag, dem 23. November 2004, um 17.30 Uhr

im Großen Hörsaal des Instituts für Experimentalphysik der Universität Wien
1090 Wien, Strudlhofgasse 4 / Boltzmanngasse 5, 1. Stock

Abstract:

With focus on computational contributions the current understanding of Brønsted acidity of zeolite catalysts is reviewed with respect to acidity strength, proton mobility, and protonation of molecules such as H_2O and CH_3OH. The mechanism of hydrocarbon transformation reactions using zeolite catalysts is not completely understood and two problems are discussed in detail in this lecture: (i) The nature of intermediates formed on the interaction of alkenes with H-zeolites or by hydride abstraction from alkanes. It is still controversial if carbenium ions are stable intermediates. As a representative example the structures and stabilities of different forms of isobutene in H-ferrierite are studied: the π-complex with the OH group (physisorption), the *primary* and the *tertiary* alkoxides and the *tertiary* isobutenium cation. Full vibrational analysis is made which permits estimates of free energies and predicts characteristic vibrational frequencies for the carbenium ion which may serve as a guide for laser spectroscopic experiments. (ii) Shape selectivity, in particular transition state shape selectivity has been proposed as a specific feature of zeolite catalysts. Computational results are presented for the m-xylene disproportionation reaction in three catalysts with different framework structures.