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Akademie věd České republiky

zve všechny zájemce na ústavní seminář, na kterém promluví

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*(Department of Chemistry,
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na téma

**„Modeling of Fuel Cell Catalysis:
Combined X-ray Photoelectron Spectroscopy,
Electrochemistry and Theoretical Studies“**

Seminář se koná **v pátek 23. března 2007 od 10.30 hod.**

ve velké posluchárně ústavu v Praze 8, Dolejškova 3.

Těšíme se na Vaši účast. Hosté jsou vítáni.



Abstract

In previous work, palladium nanoparticle catalyst was used to oxidize formic acid to CO₂ [1]. It appears that there is a correlation between the oxidation current and the core-level electron binding energy (BE) shifts of the catalyst made of different particle size. The observed BE shifts are caused by weakening of the bond strength of COOH intermediates adsorbed on the catalyst surface, which results in an increase in the oxidation rate. Overall, our measurements demonstrate a lattice strain effect - tuned by the particle size - on the electronic properties of palladium. More recently, we have shown that there is a "volcano" relationship between methanol oxidation activity and the Ru amount in Pt/Ru nanoparticle catalysts, and correlated the BE values of platinum to the reactivity. By replacing methanol to formic acid, no volcano behavior was found indicating a single, electronically controlled formic acid oxidation mechanism. The results of these studies will be reported. We will also report a combined x-ray photoelectron spectroscopy and cyclic voltammetry study of Ru(0001) electrodes modified by platinum [2]. The Ru(0001) electrodes prepared in ultra-high vacuum were covered with Pt nanoislands deposited either spontaneously or electrochemically. Pt 4f core-level BE shifts as a function of the total Pt coverage will be reported. The XPS data show that Pt 4f_{7/2} BE value decreases noticeably as the total Pt coverage increases from 0.05 to ~ 2.1 ML. The core-level BE shift is discussed in terms of the possible charge transfer and lattice strain contributions. This work highlights the significance of electronic factors in electrocatalysis, and underlines the value of theory that connects the center of the d-band shifts to catalytic reactivity.

References:

1. W. P. Zhou, A. Lewera, R. Larsen, R. I. Masel, P. S. Bagus, and A. Wieckowski, *J. Phys. Chem. B.*, **110**, 13393-13398 (2006), "Size Effects in Electronic and Catalytic Properties of Unsupported Palladium Nanoparticles in Electrooxidation of Formic Acid".
2. A. Lewera, W.-P. Zhou, R. Hunger, W. Jaegermann, A. Wieckowski and P. S. Bagus, "The Origin of Core-Level Binding Energy Shifts in Bimetallic Pt-Ru Nanoparticles", *Chem. Phys. Letters*, in preparation.

