Title:New Insights into Catalysis of Intermetallic Compounds and Porous Au

Speaker: An-Pang Tsai 蔡安邦 院士
(Institute of Multidisciplinary Research for Advanced Materials, Tohoku University)

New insights into catalysis in terms of electronic structures and microstructure have been studied. An intermetallic compound, PdZn, reveals similar valence electron density of states to pure Cu, has been testified by energy band calculation and X-ray photoelectron spectroscopy (XPS) [1]. The catalytic function was verified to be identical for the PdZn and Cu, and hence intermetallic compound like PdZn is viewed as a pseudoelement of Cu. A strong correlation between electronic structures and catalytic properties in a series of Heusler have also been verified [2].

On the other hand, we describe a new kind of low-coordinated atomic sites which can contribute to the catalytic activity of porous Au. Porous Au prepared by dealloying Al2Au exhibit high catalytic reactivity towards CO oxidation [3]. The presence of quite common twinning defects in the fcc lattice of porous Au significantly correlates with the catalytic activity. On the {211} surfaces of porous Au the twinning defects form chains of six-fold coordinated Au atoms which we denoted as W-chains. The W-chains form long rows of active Au sites. DFT calculations show that on the W-chains dioxygen chemisorbs and is activated.

[1] A.P. Tsai, et al., Acc. Chem. Res. 50(2017)2879
[2] T. Kojima et al., Sci. Adv., 4(2018)eaa6063
[3] M. Krajci, S. Kameoka, A.P. Tsai, J. Chem. Phys. 145(2016)084703

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