第314回触媒化学研究センターコロキウム

共催　電気化学会北海道支部

Rational design of electrocatalysts from material science point of view

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2012年11月15日（木）15:00−16:30

（創成科学研究棟4階セミナー室B・C）

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DFT based description of the electrocatalytic processes such as hydrogen evolution,[1] oxygen reduction,[2] or electrolytic gas[3] evolution suggests the possibility of the targeted synthesis of catalytic materials with optimized catalytic activity or selectivity. This approach represents in fact an implementation of the Sabatier principle linking the catalysts optimization of the catalytic activity with the adsorption of the catalytic process intermediate. The real catalysts design is, however, often hindered by the interdependence of two or more reaction steps when the intermediates tend to show the same linear scaling with the catalyst's reactivity which often is the only tunable parameter and thus the activity descriptor.

This drawback can be apparently addressed by modification of the active sites - small arrangements of atoms responsible for the actual catalytic activity. These sites are generally deemed to be stable and present on the catalyst's surface at all times.

A viability of these assumptions will be discussed for complex oxide and binary alloy catalysts on the basis of the information available from local structure characterization techniques. The X-ray absorption spectroscopy (XAS) data (both ex-situ and in-situ) in both XANES and EXAFS mode will be used to discuss the possibilities of targeted synthesis of oxygen evolution catalysts as well as the fundaments of the catalytic activity of the alloys in Pt-Ru or Pt-Ni systems for oxygen reduction and CO oxidation, respectively.

問合せ先：　触媒化学研究センター・大澤雅俊（osawam@cat.hokudai.ac.jp/011−706−9124）

[1] J. Greely, T. F. Jaramillo, J. Bonde, I. Chorkendorff, I., J.K. Norskov, *Nature Mater*. 5 (2006) 909.
[2] V. Stamenkovic, B. S. Mun, K. J. J. Mayrhofer, P. N. Ross, N. M. Markovic, J. Rossmeisl, J. Greeley, J. K. Norskov, *Angew. Chemie Int. Ed*. 45 (2006) 2897.
[3] Man, I. C.; Su, H.-Y.; Calle-Vallejo, F.; Hansen, H. A.; Martinez, J. I.; Inoglu, N. G.; Kitchin, J.; Jaramillo, T. F.; Norskov, J. K.; Rossmeisl, J. *Chemcatchem* 2011, 3.

314th Catalysis Research Center (CRC) Colloquium

Hokkaido Branch of The Electrochemical Society of Japan