Designing Transition Metal Oxides for Oxygen Reduction and Evolution Electrocatalysis

Jin Suntivich
Department of Materials Science and Engineering,
Cornell University, Ithaca, NY 14853

Electrocatalysis of the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) using cost-effective, abundant materials is essential for high-efficiency operation of fuel cells [1], electrolyzers [2], and metal-air batteries [3]. Transition metal oxide catalysts are possible candidates for accomplishing this task; recent studies have shown that the transition metal oxide catalysts can exhibit ORR [4] and OER [5] activities that rival the activities of the state-of-the-art precious metal-containing catalysts in alkaline environment. The high ORR and OER activities of transition metal oxides have driven many recent fundamental studies to better understand and subsequently design these materials to attain even higher ORR and OER activities [6]. In this contribution, the strategy for catalyst design inspired by a molecular orbital picture will be discussed and compared to the computational approach in the literature. Spectroscopic information to unravel the charge injection kinetics of these electrochemical reactions will also be discussed.

Reference

[1] H. A. Gasteiger, S. S. Kocha, B. Sompalli and F. T. Wagner, *Appl. Catal., B* **56** (1-2), 9-35 (2005).
[2] T. R. Cook, D. K. Dogutan, S. Y. Reece, Y. Surendranath, T. S. Teets and D. G. Nocera, *Chem. Rev.* **110** (11), 6474-6502 (2010).
[3] G. Girishkumar, B. McCloskey, A. C. Luntz, S. Swanson and W. Wilcke, *J. Phys. Chem. Lett.* **1** (14), 2193-2203 (2010).
[4] J. Suntivich, H. A. Gasteiger, N. Yabuuchi, H. Nakanishi, J. B. Goodenough and Y. Shao-Horn, *Nature Chem*. **3**, 546-550 (2011).
[5] L. Trotochaud, J. K. Ranney, K. N. Williams and S. W. Boettcher, *J. Am. Chem. Soc.* **134** (41), 17253-17261 (2012).
[6] I. C. Man, H. Y. Su, F. Calle-Vallejo, H. A. Hansen, J. I. Martinez, N. G. Inoglu, J. Kitchin, T. F. Jaramillo, J. K. Norskov and J. Rossmeisl, *ChemCatChem* **3** (7), 1159–1165 (2011).