Combinatorial Experimental and Theoretical Search Strategies for new Fuel Cell Catalysts

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Combinatorial high-throughput experimentation and predictive theoretical modeling represent very different, yet, when combined, very powerful screening methods in materials science for rapid mapping of activity-property relationships within the materials landscape.

Here, we present a comparative study of search strategies based on combinatorial electrochemical screening and predictive model calculations using density functional theory (DFT). Both methods were applied to the discovery of new ternary alloy catalysts for PEM fuel cell anodes of improved activity and tolerance towards surface poisons. Strengths and limitations of the two screening strategies are discussed, and anode catalyst compositions identified by either method are compared.

In the combinatorial experimental study [1], 64-element material libraries of well-defined thin-film electrocatalysts were prepared using vacuum deposition techniques. Diverse multi-metal library designs as well as focused library designs were used to map activity-composition relationships and to pin down portions of compositional space of high catalytic activity. All 64 catalysts were screened in parallel for activity towards electro oxidation of methanol in acidic electrolytes.

In the theoretical studies, DFT calculations were used to describe the adsorption of CO and H_2O on close packed alloy surfaces [2,3]. The calculated adsorption energies were used as input into a simple kinetic model at conditions relevant to the anode of a PEM fuel cell. The model allowed analyzing the origin of the promoting effect a Pt-alloy surface relative to pure Pt.

[1] Strasser, P.; Gorer, S. and Devenney, M. in *Direct Methanol Fuel Cells***,** S.R. Narayanan,S. Gottefeld, T. Zawodzinski,eds., ECS Proceedings Volume 4, 2001, p.191

[2] P. Liu J.K. Norskov Fuel Cells 1 (2001) 192

[3] P. Liu, A. Logadottir and J.K. Norskov, preprint