Mesoscale Priority Research Direction

Microcatalyst Engineering

Opportunity

Metallic mesoscale materials show promise for diverse energy electrocatalysis applications, including fuel cell and electrolyzer catalyst materials. Precious metals such as Pt, Pd, Ir, and Au possess high catalytic activity, and galvanic displacement reactions have been demonstrated to synthesize mesoscale structures of these materials. A better understanding of galvanic displacement reaction will expand a large design space for these electrocatalyst materials.

Approach

Spontaneous galvanic displacement is a mechanism in which a "less noble" metal acts simultaneously as a sacrificial template and a reducing agent, resulting in spontaneous electron transfer to and deposition of an oxidizing or "more noble" metal. For example, Pt nanowire electrocatalysts may synthesized by galvanic displacement of Ag nanowires. A conceptual model and design tools are needed to understand the diversity of observed products. Adaptation of high-performance computing frameworks and correlation with results from advanced experimental techniques is required.

Meso Challenge

Modeling of collective electrodeposition, corrosion, and morphogenetic phenomena in mesoscale materials requires coupling quantum and classical phenomena, from surface diffusion kinetics through nanoscale structure formation to mesoscopic structure of catalyst particles.

Impact

A combination of experimental and simulation workflows probing atomic through mesoscale phenomena would allow systematic exploration of catalyst design spaces with greater confidence. Successful design would bring down electrocatalyst costs, aiding the eventual widespread adoption of energy technologies such as fuel cells and electrolyzers.

References:

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2. Nørskov, J.K., et al. (2011) *Proc. Natl. Acad. Sci. USA* **108**: 937-43

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Contact: Christopher Chang, Bryan Pivovar, Brian Larsen (NREL)