LA-SiGMA

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Nanoporous Metal Catalysts: Synthesis, Activity, and Stability

by

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The improvement of the catalytic efficiency for the oxygen reduction reaction (ORR) is one of the most important challenges in low-temperature fuel cell technology. Platinum is the most active element for the ORR but its high cost and scarcity hinder the commercial implementation of fuel cells in automobiles. Pt-based alloys are promising alternatives to substitute platinum while maintaining the efficiency and life-time of the pure catalyst. However, the presence of an acid medium and oxidation of the surface impacts the activity and durability of the alloy catalysts through changes in its local composition. Dealloying is the selective removal of elements from an alloy. According to recent experimental reports dealloying taking place during the synthesis of ORR catalysts may yield remarkable activity enhancement by creating characteristic porous or hollow structures. However, the dealloying process that occurs during the fuel cell operation is enhanced by the concomitant presence of oxygen that promotes metal dissolution causing the degradation of the catalyst. In this work the driving forces and the effect of dealloying on the structure of ternary alloy nanocatalysts during their synthesis and operation are studied with a multi-scale approach including density functional theory, molecular dynamics, and Kinetic Monte Carlo simulations.

Dr. Perla B. Balbuena graduated as Ingeniera Química at Universidad Tecnológica Nacional, Facultad Regional Rosario, Argentina. She received a Master in Science degree from the University of Pennsylvania and a PhD degree from the University of Texas at Austin, both in chemical engineering. Her PhD dissertation investigated the effects of water as a solvent at high pressures and temperatures on chemical reactions, using molecular simulation techniques. Dr. Balbuena was Assistant Professor from 1997 to 2002 and Associate Professor from 2002 to 2004 at the University of South Carolina, Department of Chemical Engineering. Since 2004, she is Professor of Chemical Engineering, and Professor of the Materials Science and Engineering Program at Texas A&M University. Her research focuses on first-principles computational design of materials and processes. In recent years, she has been active in the field of materials design with applications to electrolytes and electrodes of lithium-ion batteries and fuel cells, catalyzed growth of single-walled carbon nanotubes, hydrogen storage, and gas separations using porous materials. She has published one hundred and sixty nine peer-reviewed articles and has been co-editor of five books in her fields of specialization.