Title
Catalytic materials for energy conversion and storage: From theory to product

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Abstract: In this presentation, a research system that connects fundamental investigation on well-defined extended surfaces (e.g. single crystal surfaces), theoretical studies using computer-powered simulation, and finally design of high performance catalysts in which all the possible beneficial properties from complex functional structures are implemented, will be demonstrated.Control of structure at the atomic level can precisely and effectively tune catalytic properties of materials, enabling enhancement in both activity and durability. To mimic the optimal surface structure of Pt3Ni(111)-Pt-Skin for oxygen reduction reaction (ORR), a highly active and durable class of electrocatalysts are prepared by exploiting the structural evolution of Pt-Ni bimetallic nanocrystals. The starting material, crystalline PtNi3 polyhedra, transformed in solution by interior erosion into Pt3Ni nanoframes with surfaces that have three-dimensional molecular accessibility. The edges of these PtNi3 polyhedra, which were Pt rich, are maintained in the final Pt3Ni nanoframes. Both the interior and exterior catalytic surfaces of this open framework structure are composed of the nano-segregated Pt-Skin structure that exhibits enhanced oxygen reduction reaction (ORR) activity. The Pt3Ni nanoframe catalysts achieved over 36 and 22-fold enhancement in mass and specific activities, respectively, for this reaction versus ORR in comparison to state-of-the-art Pt/C catalysts during prolonged exposure to reaction conditions.Notes and references: Stamenkovic et al. Science 315, 493-497 (2007). Kang et al. Science DOI: 10.1126/science.1249061 (2014).

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