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Jane Tierney
Scientific & Technical Information
Manager

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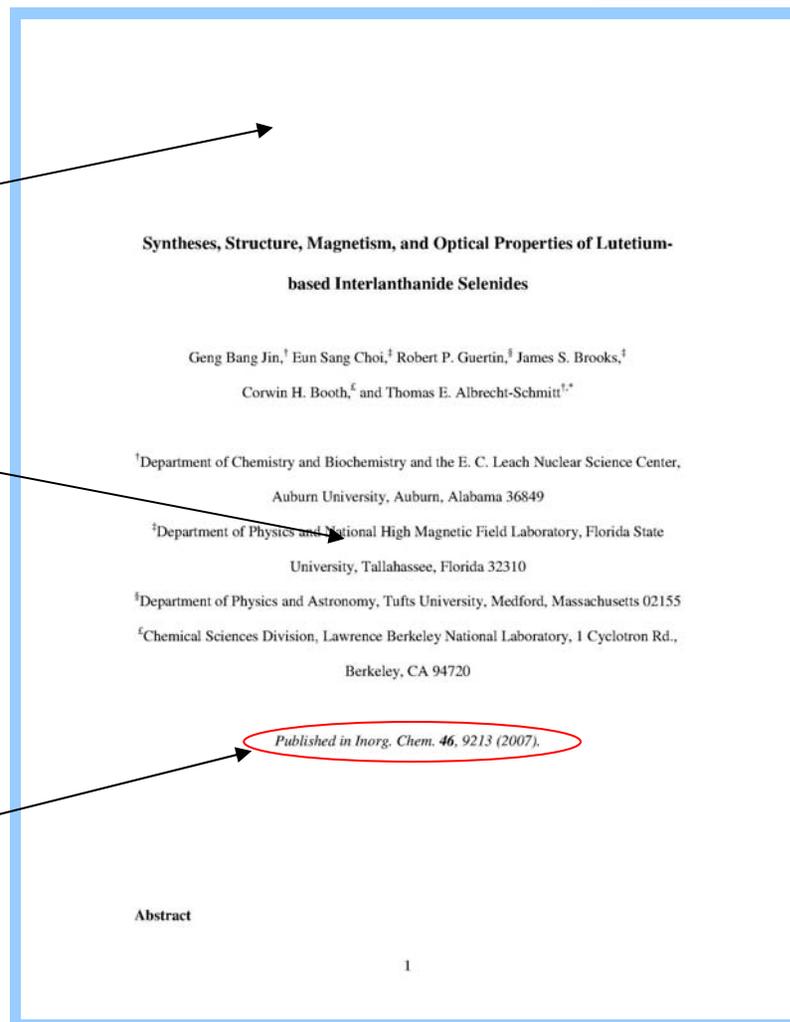
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ARTICLES

Trends in electrocatalysis on extended and nanoscale Pt-bimetallic alloy surfaces

VOJISLAV R. STAMENKOVIC^{1,2*}, BONGJIN SIMON MUN^{2,3}, MATTHIAS ARENZ⁴, KARL J. J. MAYRHOFER⁵, CHRISTOPHER A. LUCAS⁵, GUOFENG WANG⁵, PHILIP N. ROSS² AND NENAD M. MARKOVIC^{1*}

¹Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA
²Materials Sciences Division, Lawrence Berkeley National Laboratory, University of California, Berkeley, California 94720, USA
³Department of Applied Physics, Hanyang University, Ansan, Kyunggi-Do 426-791, Korea
⁴Technical University of Munich, 85333 Munich, Germany
⁵Oliver Lodge Laboratory, Department of Physics, University of Liverpool, Liverpool L69 7ZE, UK
⁶Department of Chemistry and Physics, University of South Carolina, Aiken, South Carolina 29801, USA
*e-mail: vrstamenkovic@anl.gov; nmmarkovic@anl.gov

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One of the key objectives in fuel-cell technology is to improve and reduce Pt loading as the oxygen-reduction catalyst. Here, we show a fundamental relationship in electrocatalytic trends on Pt₁M (M = Ni, Co, Fe, Ti, V) surfaces between the experimentally determined surface electronic structure (the *d*-band centre) and activity for the oxygen-reduction reaction. This relationship exhibits 'volcano-type' behaviour, where the maximum catalytic activity is governed by a balance between adsorption energies of reactive intermediates and surface coverage by spectator (blocking) species. The electrocatalytic trends established for extended surfaces are used to explain the activity pattern of Pt₁M nanocatalysts as well as to provide a fundamental basis for the catalytic enhancement of cathode catalysts. By combining simulations with experiments in the quest for surfaces with desired activity, an advanced concept in nanoscale catalyst engineering has been developed.

The development of new materials that can solve challenging problems in the areas of clean energy production, conversion and storage is of paramount importance in the quest to find an alternative to environmentally unfriendly fossil-fuel use. One promising alternative is the polymer electrolyte membrane fuel cell¹⁻⁴, a device in which hydrogen, through its reaction with oxygen, produces water as its only product. To make hydrogen-based energy systems a vibrant and competitive force, many problems still need to be solved⁵; the main one being to find a more effective catalyst than Pt for the oxygen-reduction reaction (ORR), the cathodic half-cell reaction in the hydrogen-oxygen (air) fuel cell ($1/2\text{O}_2 + 2\text{H}^+ + 2\text{e}^- = \text{H}_2\text{O}$).

Electrocatalysts with unique properties can be created by alloying two or more metals. Several investigations⁶⁻¹¹ have been carried out to determine the role of alloying in the electrocatalytic activity of Pt for the ORR; a definitive determination, however, remains elusive. For example, a series of binary PtM alloys (M = Cr, Mn, Co, Ni) supported on carbon produced some enhancement in the kinetics of the ORR (a factor of 3–5, ref. 12) relative to 'standard' supported Pt catalysts. One of the difficulties in determining the effect of alloying using supported catalysts, however, is that the activity of a supported catalyst can have a wide range of values depending on its microstructure and/or method of preparation. The intrinsic activity of nanoparticles depends on particle size, shape and composition¹⁰; that is, there is no single value of the specific activity even when normalized by Pt surface area. As the alloyed catalyst particles may not have either the same particle size or shape as the Pt catalysts with which they are compared, a simple comparison of activity

normalized either by mass or surface area is insufficient to identify a true alloying effect. Furthermore, because both the surface segregation and segregation-induced changes in the surface electronic properties are unknown for Pt-bimetallic nanoparticles, the effect of chemical composition and/or atomic/electronic surface structure on reactivity is still unresolved. These complexities regarding supported catalysts emphasize the need for using well-characterized materials to identify the fundamental mechanisms at work in the ORR.

Here, emphasis is placed on advanced concepts that can be used to understand and predict variations in the ORR reactivity caused by the effects of alloying Pt with the 3d-transition metals. Electrocatalytic trends in the ORR are established as a relation between the surface composition, specific activity (kinetic current density, i_k) and the surface electronic structure of Pt₁M (M = Ni, Co, Fe, V, Ti) alloy surfaces.

Before exploring trends in catalytic activity, it is important to describe, briefly, the ultrahigh-vacuum (UHV) methodology used to prepare (sputtering/annealing cycles) and to characterize the cleanliness (Auger electron spectroscopy, AES), the composition of the surface atomic layer (low-energy ion scattering, LEIS) and the electronic surface structure (ultraviolet photoemission spectroscopy, UPS) of the Pt₁M alloy surfaces. As the preparation/characterization methodology is the same for all Pt₁M alloys^{13,15}, the results for Pt₁Fe are described as a representative case. AES spectra of Pt₁Fe, shown in Fig. 1a, reveal that after sputtering/annealing cycles, the surfaces are free of impurities such as C and O. The Pt/Fe AES peak ratio is reduced on a sputtered surface compared with an annealed surface. This was the first

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