Experimental and Theoretical Studies of Cathode Electrocatalysts for Fuel Cells

Frontiers in Catalysis Science and Engineering Seminar Series

Presented by…

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Abstract: Recently our research group has performed experimental and theoretical studies of the novel catalytic and electrocatalytic properties Pt-based bimetallic alloys, in particular the subsurface Pt-3d-Pt (3d = Ni, Co, Fe) structures [1-3]. Our research approaches are aimed at bridging the "materials gap" and "pressure gap" using a combination of DFT calculations, UHV studies on single crystal and polycrystalline surfaces, and reactor and fuel cell studies of supported catalysts. In the current talk we will present our recent results on the advantages and challenges of using Pt-3d-Pt as cathode electrocatalysts for PEM fuel cells.

We will first correlate the enhanced Oxygen Reduction Reaction (ORR) activity with the binding energy of atomic oxygen on different bimetallic surfaces. We will then address the most critical question for the application of Pt-3d-Pt for ORR application, *the stability of the subsurface structure in the presence of adsorbed oxygen*. We will provide DFT calculations of the thermodynamic stability and experimental measurements of the segregation kinetics of subsurface 3d atoms in the presence of oxygen on single crystal Pt-3d-Pt(111) structures. These results will be correlated with segregation kinetics of the corresponding bimetallic structures on polycrystalline films, measured both under UHV [4,5] and atmospheric [6] conditions. We will also confirm the segregation and dissolution of subsurface 3d metals using an electrochemical half cell that is attached to a UHV system. Finally, we will propose the possibility to overcome the intrinsic instability of the Pt-3d-Pt structure by anchoring the subsurface 3d atoms on the substrates of transition metal carbides.

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Wednesday
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ETB Columbia River

9:00 – 10:00 am

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