Experimental and Theoretical Studies of Novel Electrocatalysts for Fuel Cells

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Metal carbides [1-3] and bimetallic alloys [4-7] often show novel catalytic and electrocatalytic properties. However, it is difficult to know *a priori* how the chemical properties of particular carbide and bimetallic systems will be modified relative to the parent metals. In the past few years our research group has investigated the novel catalytic properties of various carbide and bimetallic systems, using a combination of Density Functional Theory (DFT) calculations, surface science studies on single crystal surfaces, and reactor and fuel cell studies of supported catalysts. The general trends from the experimental and theoretical studies of carbide [1] and bimetallic surfaces [4] have been summarized in recent reviews.

In the first part of the talk we will describe the utilization of tungsten carbides as potential anode electrocatalysts for Direct Methanol Fuel Cells (DMFC). Currently, the anode electrocatalysts for DMFC are Pt and Pt/Ru, which are disadvantageous in terms of the prohibitively high costs and their susceptibility to be poisoned by CO. We will describe how to control the decomposition pathways of methanol on single crystal surfaces of tungsten carbides under well-controlled ultrahigh vacuum (UHV) conditions. We will also discuss the synthesis of phase pure tungsten carbide electrodes using Physical Vapor Deposition (PVD) to bridge the "materials gap" between single crystal surfaces and polycrystalline films. We will then present our results of the electrochemical evaluation of the tungsten carbide electrodes to bridge the "pressure gap" between UHV environment and electrochemical conditions. In the second part of the talk we will discuss the thermodynamic stability and kinetic measurements regarding the bimetallic surfaces in the presence of oxygen under both UHV [8] and atmospheric [9] conditions, which should help identify active and stable bimetallic cathode electrocatalysts in the Oxygen Reduction Reaction (ORR) in fuel cells.

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