Oxygen Reduction Reaction on Non-Platinum Fuel Cell Cathodes

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Platinum has widely been used as the electrode material in low-temperature polymer electrolyte membrane fuel cells (PEMFCs) due to its efficiency in catalyzing the hydrogen dissociation and oxygen reduction reaction (ORR) (Figure 1). However, the high price of platinum-based catalysts makes PEMFCs very expensive. One of the alternative ways is to use non-platinum catalytic materials instead. Unfortunately, the experimental chemists haven't been able to get improved catalytic activity with non-platinum pure metal nano-particles. Here we present results of our systematical computational investigation of the reaction mechanism and corresponding reaction barriers using quantum mechanics periodic slab calculations. The calculated pure platinum surface and four non-platinum metal surfaces can be categorized into two types: platinum-like and palladium-like metals. Metals within each type have a similar surface site selection rule when binding with hydrogen, oxygen and other oxygen-containing species involved in the ORR. Consequently, the two types of the metals have different reaction mechanisms.

Figure 1. Oxygen reduction reaction on Pt surface.