

ACTIVE SITES FOR PEM FUEL CELL REACTIONS

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INTRODUCTION

The development of electrocatalytic materials of enhanced activity and efficiency through careful manipulation, at the atomic scale, of the catalyst surface structure, has long been a goal of electrochemists.

To accomplish this ambitious objective, it would be necessary to obtain a thorough understanding of the relationship between the atomic-level surface structure and the catalytic properties.

In the past, the most common approach for establishing structure function relationships was to correlate electrochemical behavior of different single crystal surfaces, assuming perfectly ordered surfaces.

In this work, however, we focus on the sub-structures which exist on single crystal surfaces. Using sample preparation and characterization (STM, FT-IRAS and SXS) methods of metal single crystal surfaces, we were able to monitor and control adsorbate-/ potential-induced changes in the coordination of surface atoms. This, in turn, allowed us to find correlations between the nature as well as the number of active sites and the rate of PEM-FC reactions.

In combination with theoretical techniques (DFT calculations), we were also able to find a possible explanation for the enhanced activity at the active sites.

The knowledge about the active sites for a particular reaction is a prerequisite and the first step to understanding how to tune a catalyst performance.

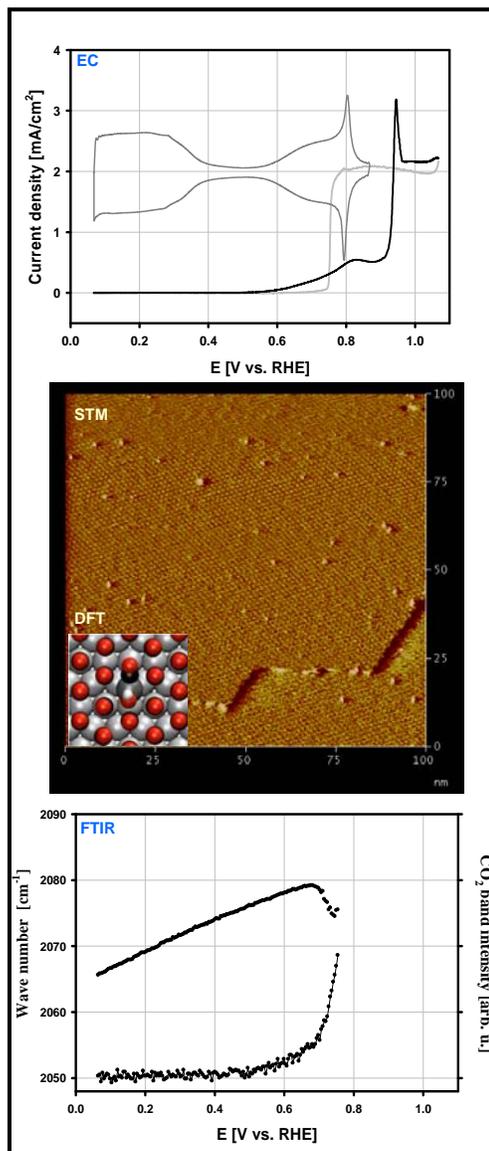
RESULTS

In the case of CO oxidation on platinum, the results show that the ad-islands exhibit a unique activity and can be stabilized under conditions relevant to this reaction.

DFT calculations suggest that the enhancement in activity comes from favorable competition of OH with CO for sites on adatoms in CO-saturated solutions in comparison to perfect terraces.

By increasing the amount of the active sites by means of preparation procedure, we were able to tune platinum activity for CO oxidation to the level of the most active alloy catalysts.

Furthermore, we implemented the knowledge on single crystals to real systems, obtaining a catalyst with several orders of magnitude higher activity than commercially available platinum catalysts.



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