



Theory and Experiment in Electrocatalysis (Modern Aspects of Electrochemistry)

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Electrocatalysts are the heart of power devices where electricity is produced via conversion of chemical into electrical energy. - pressive advances in surface science techniques and in first pr- ciples computational design are providing new avenues for signi- cant improvement of the overall efficiencies of such power dev- es, especially because of an increase in the understanding of el- trocatalytic materials and processes. For example, the devel- ment of high resolution instrumentation including various electron and ion-scattering and in-situ synchrotron spectroscopies, elect- chemical scanning tunneling microscopy, and a plethora of new developments in analytical chemistry and electrochemical te- niques, permits the detailed characterization of atomic distribution, before, during, and after a reaction takes place, giving unpre- dented information about the status of the catalyst during the re- tion, and most importantly the time evolution of the exposed ca- lytic surfaces at the atomistic level. These techniques are c- plemented by the use of ab initio methods which do not require input from experimental information, and are based on numerical solutions of the time-independent Schrodinger equation including electron-electron and electron-atom interactions. These fir- principles computational methods have reached a degree of - turity such that their use to provide guidelines for interpretation of experiments and for materials design has become a routine practice in academic and industrial communities.

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