

Abstract Submitted  
for the MAR06 Meeting of  
The American Physical Society

**Modeling Electrocatalysis – Electro-oxidation of Pt(111)** TIMO JACOB, MATTHIAS SCHEFFLER, Fritz-Haber Institute, Faradayweg 4-6, D-14195 Berlin, Germany — Electrochemical reactions (such as in fuel cells) usually occur under conditions of finite temperature, pressure, and electrode potential, implying a very involved situation, possibly leading to novel surface materials. Especially the presence of an electrode potential, which results in the formation of an electric double-layer, affects the composition and structure of the electrode/electrolyte-interface. Towards a more realistic treatment of electrocatalysis we developed an appropriate theory in which the electrode of the interface is assumed to be in contact with a *bulk-electrode* reservoir (at chemical potential  $\mu_{el}$ ) while the electrolyte is in contact with a *bulk-electrolyte* reservoir. Although we are in the process of simulating the entire electric-double layer self-consistently, the present approach already allows us to estimate the limites of the expected effects. As a first application we studied the electro-oxidation of Pt(111) by calculating the  $p/T/\phi$ -phase diagram. The obtained behavior, that positive electrode potentials stabilize higher oxygen coverages, is in qualitative agreement with cyclic-voltammetry experiments.

Timo Jacob  
Fritz-Haber Institute, Faradayweg 4-6, D-14195 Berlin, Germany

Date submitted: 28 Nov 2005

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