Modeling Electro catalysis – 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 limits 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          Electronic form version 1.4