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 electro-catalysis 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/φ-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

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