RUHR-UNIVERSITÄT BOCHUM

RESOLV
RUHR EXPLORES SOLVATION
CLUSTER OF EXCELLENCE - EXC 1069

RUB

SEMINAR ANNOUNCEMENT

THURSDAY, 05.07.2018
14:00 h ZEMOS 0.17

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"Structures of electrode-electrolyte interfaces studied from first principles"

In recent years, there has been significant progress made in the modeling of electrochemical interfaces and electrocatalytic processes from first principles. Trends in the electrocatalytic activity have been addressed and understood in terms of simple, but powerful reactivity concepts. However, in many of the computational studies, the influence of the electrochemical environment has not explicitly been into account. Thus the role of the explicit presence of the electrolyte, the correct equilibrium electrode coverage of ions from the solution and/or the influence of varying electrode potentials on electrocatalytic processes still need to be assessed.

In this presentation, I will show how the equilibrium coverage of hydrogen and halides on metal electrodes can be addressed based on a grand-canonical scheme. The presence of the electrolyte is treated either implicitly or explicitly and/or as a thermodynamic reservoir for solvated species. Furthermore, I will address dendrite formation at battery electrodes which can form a significant hazard in battery operation. I will discuss whether chemical trends in the dendrite growth can be derived based on the height of metal self-diffusion barriers

Guests are very welcome!