Insights into electrochemical problems from the perspective of semiconductor defect chemistry

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Ab initio simulations provide detailed insights into the atomic scale and have proven indispensable in aiding the study of problems in diverse areas of materials science related to metals, ceramics, semiconductors or functional materials. In the last years, ab initio based simulations of electrochemical processes have experienced an enormous methodological development. These allow the description and study of stability and reactivity of solid/liquid interfaces at the computer in dependence of the environmental conditions, as dictated by the *p*H-value of the solution and the applied electrode potential.

During the lecture, I will discuss an approach we developed recently, which unifies and "translates" theoretical concepts from the areas of semiconductor defect chemistry and electrochemistry [1]. This approach is based on a fully grand-canonical description of both ions and electrons, linking ab initio calculations quite naturally to experimental observables such as the *p*H-scale and the electrode potential. It provides new insights into apparently "old" problems such as water stability or oxide growth in an corrosive environment, opens new routes to construct electrochemical phase (Pourbaix) diagrams and gives a handle to an absolute alignment of electrochemical potentials.

References:

[1] M. Todorova und J. Neugebauer, Phys. Rev. Appl. **1**, 014001 (2014).
[2] M. Todorova und J. Neugebauer, Surf. Sci. **631**, 190-195 (2015).
[3] M. Todorova und J. Neugebauer, Farad. Discussions **180**, 97-112 (2015).
[4] A. K. Vatti, M. Todorova and J. Neugebauer, Langmuir **32**, 1027 (2016).