

Extending thermodynamic concepts combined with first-principles calculations to address questions related to aqueous corrosion: potential and challenges

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The ability to predictively characterise the plethora of elementary processes contributing to the corrosion of materials will greatly enhance our understanding of the functionality of a corrosion cell and aid systematic improvement of corrosion protection, which is often a question of trial and error approaches, largely based on empirical observations rather than sound theoretical understanding.

A meaningful investigation of such elementary processes requires the accuracy of a quantum mechanical description, but the prominent role which water plays in a corroding system makes theoretical modelling rather challenging. I will discuss our use of first principles calculations combined with thermodynamic considerations to address questions relevant to corrosion. By extending thermodynamic concepts routinely used in the realm of surface science we can understand the stability of ZnO(0001) surfaces in dry and humid atmosphere [1,2], while an approach derived from the defect chemistry of semiconductors enables us to link the electrode potential and the pH-scale seamlessly to *ab-initio* calculations. This method is based the formation energy of ions in an aqueous host matrix and will, depending on our ability to obtain accurate ion hydration energies, allow us to exploit the advantages of *ab initio* calculations to address key questions in electro-chemistry.

[1] M. Valtiner, M. Todorova, G. Grundmeier, and J. Neugebauer, Phys. Rev. Lett. **103**, 065502 (2009).

[2] M. Valtiner, M. Todorova, and J. Neugebauer, Phys. Rev. B **82**, 165418 (2010).