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LECTURE

**“Electrochemical energy conversion and storage from a
first-principles point of view”**

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NHRF

Electrochemical energy conversion and storage from a first-principles point of view

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In order to improve the efficiency of electrochemical energy conversion and storage, an atomistic understanding of the elemental (electro-)chemical processes can be rather helpful. However, a quantum chemical first-principles' description of electrochemical electrode-electrolyte interfaces is hampered by the complexity of these system involving liquid electrolytes and varying electrode potentials.

In this talk I will show how in a step-wise approach the electrochemical environment can be taken into account in order to study electrocatalytic processes theoretically [1,2]. Furthermore, the origins of dendrite growth in batteries which represents a significant hazard in battery operation will be discussed. It will be proposed that the height of self-diffusion barriers can be used as a descriptor for the occurrence of dendrite growth [3].

References

- [1] T. Roman and A. Groß, ACS Catal. **6**, 5575 (2016).
- [2] F. Gossenberger, T. Roman, and A. Groß, Electrochim. Acta **216**, 152 (2016).
- [3] M. Jäckle, K. Helmbrecht, M. Smits, D. Stottmeister, and A. Groß, Energy Environ. Sci., doi: 10.1039/C8EE01448E