UNIVERSITÄT DUISBURG ESSEN

Offen im Denken

Theorie-Kolloquium WS 2021/22

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Electrified surfaces at constant electrode potential: an ab initio perspective

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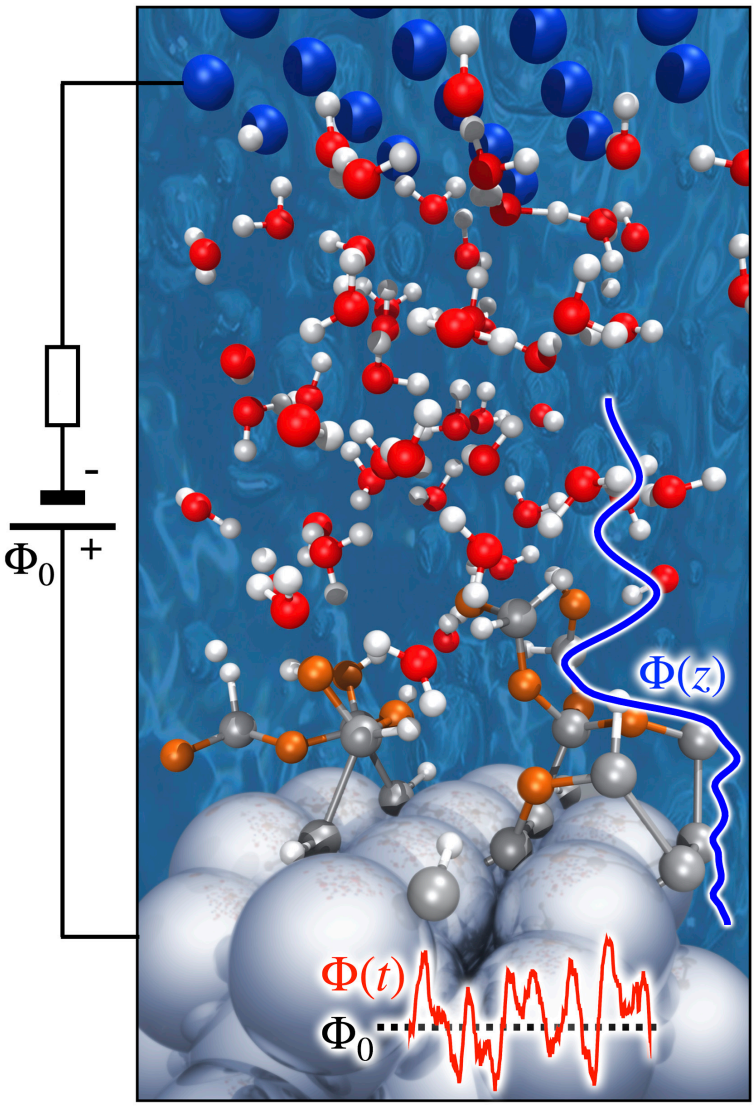
Developing accurate simulation techniques to explore and predict structural properties and chemical reactions at electrified surfaces in contact with liquid electrolytes will be critical to surmount materials-related challenges in the context of energy conversion and storage. Exciting progress in recent years allows us now to realistically describe electric fields at charged surfaces from first principles. Building on these techniques, we recently introduced a “thermopotentiostat”: a novel approach to control the electrode potential in ab initio molecular dynamics (AIMD) simulations. Our thermopotentiostat approach can be straightforwardly implemented into any density-functional code. In this talk, we will provide a brief perspective on the key concepts of AIMD simulations at controlled electrode potential. To highlight the opportunities provided by these developments we discuss the dielectric response and splitting of liquid water in contact with electrified semiconductor surfaces.



F. Deißenbeck, C. Freysoldt, M. Todorova, J. Neugebauer, S. Wippermann, PRL 126, 136803 (2021)