

## **Insights into processes at solid/liquid interfaces from ab initio molecular dynamics simulations**

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Processes at the solid/liquid are at the heart of many present day technological challenges related to the improvement of battery materials, electro-catalysis, fuel cells, corrosion and others. Understanding and quantifying the underlying fundamental mechanisms will enable targeted design of desired functionalities, but is equally challenging to theoretical modelling and experimental characterisation.

Recently we developed a novel potentiostat design [Surendralal *et al.*, Phys. Rev. Lett. **120**, 246801 (2018)] and a canonical thermopotentiostat [Deißbeck *et al.*, Phys. Rev. Lett. **126**, 136803 (2021)] approach, in which the electrode potential of the system is controlled by tuning the excess charge of the working electrode. This enables us to study solid/liquid interfaces under realistic conditions of applied bias by ab-initio molecular dynamics simulations and obtain direct insight into key mechanisms of electrocatalysis and corrosion. The study of the H/Pt/H<sub>2</sub>O system provides valuable insights into the role of the solvent on the workfunction evolution at metal/electrolyte interfaces [Surendralal *et al.*, Phys. Rev. Lett. **126**, 166802 (2021)]. Applying bias to Mg/water interfaces allows us to elucidate the mechanism underlying the experimentally observed link between H-evolution under anodic conditions and Mg dissolution.