THEOS
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MARVEL
NATIONAL CENTRE OF COMPETENCE IN RESEARCH

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

Computational Simulations of the Electrochemical Interface at the Atomic Scale

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Abstract: The electrochemical interface is a key element of various systems such as energy-conversion devices, biochemical sensors, transistors, catalytic processes… It is thus important to develop computational approaches that can assist experimental work in understanding and improving interfacial designs and mechanisms at the atomic scale.
In this talk, I will present a few contributions in developing a self-consistent picture of the electrochemical interface where the effects of potential, charge, adsorption isotherms, surface stability, solvent, and ionic strengths are intertwined. Also, in complement to mean-field screening approaches, the possible need to account for dynamical and transient effects will be illustrated.