THEOS
THEORY AND SIMULATION OF MATERIALS

MARVEL
NATIONAL CENTRE OF COMPETENCE IN RESEARCH

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Advances in Continuum Embeddings for Electrochemistry

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Abstract: Continuum models of solvation have played a crucial role in the computational characterization of molecules solvated in neutral or electrolyte solutions. Recent advances in the field have extended the capabilities of this class of methods towards the characterization of solvated interfaces, possibly in the presence of an applied electrochemical potential. These recent advances have opened the possibility of modeling heterogeneous catalysis and electrochemistry in a first-principles-based framework, where the multiscale nature of the developed approaches provides a significant reduction of the computational burden while retaining a good accuracy. Moreover, recent improvements in the definition of continuum interfaces have allowed to overcome fundamental limitations of these approaches, opening the way for new applications. Here the core methodological aspects and the most recent features of these recently developed continuum solvation approaches, as implemented in the ENVIRON library (www.quantum-environ.org), will be reviewed. Applications to the study of environment effects on materials, including recently proposed 2D materials, will be presented.