

Mechanistic investigations at the solid/water interface

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Reactions at the water/solid interface are central to develop more sustainable processes, from biomass upgrading to the use of unconventional activation as in photocatalysis and electrocatalysis. To gain atomistic insight on those reactions, modelling approaches were constantly improved in the past decade. Several approaches are available nowadays from continuum models to a full explicit description of the liquid water.¹ We will discuss the pros and cons of those methods using several examples.

Keywords: DFT ; ab initio molecular dynamics ; Solvent effect ; Catalysis

¹ Steinmann, S. N. & Michel, C. How to Gain Atomistic Insights on Reactions at the Water/Solid Interface? *ACS Catalysis*, **2022**, *12*, 6294-6301