

Modeling reactivity at the catalyst/water interface

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To describe reactions occurring at the solid/water interface is currently one of the major challenges in modeling in Heterogeneous Catalysis, especially in the context of biomass valorization.[1] It requires a proper depiction of the water solvent together with an adequate description of the surface state. Several approaches are available nowadays in the literature, from continuum models to a full explicit description of the liquid water.[2] When H-bonding between the liquid water and the reactant or intermediate is crucial, continuum models are not sufficient and an explicit inclusion of water molecule is a necessity. As a first step, micro-solvation can be an effective approach that allowed us to interpret solvent effect in the conversion of levulinic acid into γ -valerolactone.[3] Moving to a full description of reactivity the water/metal interface is still beyond a full complete DFT approach provided the minimal size of the periodic cell that is necessary and the minimal sampling required. A combined QM/MM approach could be a promising strategy,[4] but necessitates a new generation of metal/water force field.[5] Nevertheless, being less demanding, inspecting transformations occurring at oxide/water interface is now reachable, as illustrated by our recent work on the stability of γ -alumina in water. After a fine characterization of the interfacial water[6], we located the weak spot on γ -alumina by a combination of experimental reactivity of shaped-controlled crystals and metadynamics simulations and finally provided a rationale for the greatest stability in presence of C5 and C6 polyols.[7]

References

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