Dynamic Modelling of Active Sites in Heterogeneous Catalysis

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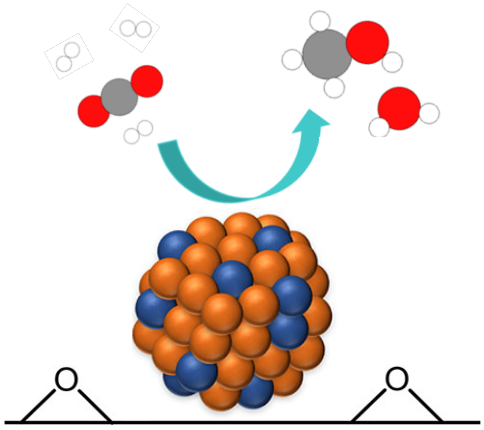
Abstract: Theoretical calculations can provide unique information about how heterogeneous catalysts work at the atomic level. Nevertheless, modeling these materials is highly complex since many processes interplay at different spatial-temporal scales. Moreover, catalysts are "alive," containing potentially dynamic active sites, impacting their overall performance. Present theoretical methods do not fully capture their complexity and are computationally intensive, hampering the theory-based design of better catalytic materials.

This talk will show our recent works to understand heterogeneous catalysts via a computational approach, focusing primarily on CO/CO_2 conversion processes catalyzed by metal-based systems.[1-5] We will discuss the active sites of the materials and their intrinsic activity,[1] how to simulate them at different time and length scales,[2] and screen their reactivity faster.[3] Showcase systems modeled via a static[5,6] and a dynamic approach will also be presented. Finally, we will cover our ongoing and envisioned work to improve theoretical techniques to comprehend heterogeneous catalyst dynamics better.



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