

## **Operando modeling of functional nanostructured materials for sustainable chemistry, nanosensing and clean energy**

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Within this talk, I will illustrate how we can model functional nanostructured materials for sustainable chemistry, nanosensing and clean energy at operando conditions, mimicking as close as possible the experimental conditions to enable future technological solutions. Our society is confronted with important challenges, such as how can we provide an affordable and clean energy system without endangering future generations, how can we protect our limited natural resources, how can we combat environmental pollution, how can we mitigate climate change. Functional nanomaterials play a pivotal role in the development of future technological solutions to provide answers to these questions. From a purely experimental basis, it is extremely difficult to establish a causal relation between nanometer scale structural modifications and the observed macroscopic function of the material. Modeling functional nanomaterials in close synergy with experiment has the potential to give this nanoscopic insight, provided it yields a realistic nanometer scale representation of the functional material.

Nanostructured materials used in applications are far from perfect, they possess a broad range of heterogeneities in space and time extending over several orders of magnitude. Spatial heterogeneities from the subnanometer to the micrometer scale in crystal particles with a finite size and specific morphology, impact the material's dynamics. Furthermore, the material's functional behaviour is largely determined by the operating conditions. Currently, there exists a huge length-time scale gap between attainable theoretical length-time scales and experimentally relevant scales. Within this talk I will give an overview of the current state of the art in modelling functional nanostructured materials and challenges yet to be overcome to model nanostructured materials to mimic as close as possible experimental conditions.

The concepts will be made clear by timely applications in the fields of sustainable chemistry, clean energy and nanosensing. Materials and applications encompass zeolites to convert non-fossil based feedstocks like biomass, C1 molecules to useful building blocks for the chemical industry; stimuli-responsive metal-organic frameworks that respond upon multiple triggers (mechanical, gas adsorption, electric fields); metal halide perovskites with an optical function to efficiently utilize solar energy for chemical conversions or energy harvesting.

It will become clear how modeling in close synergy with experiment is quintessential in understanding the function of nanostructured materials. I will show some of our recent endeavors to drastically extend accessible length and time scales in molecular modeling using machine learning techniques and molecular dynamics techniques.