Multiscale Modelling : An Industrial Perspective

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Abstract

Computational techniques to model material properties and catalytic behaviour have now become mainstream tools in an industrial setting. This is due to two main factors: improved algorithms that accurately model material behaviour and increased computational power enabling faster simulations. As such, multi-scale simulations, ranging from electronic structure to continuum-based approaches have become embedded in product development cycles, innovating the way in which new products are developed.

The talk will give an overview of how multi-scale modelling combined with advanced characterization techniques are being used in industry to understand the structure and activity of catalytic materials that are used to accelerate the transition to net zero. Multi-scale modelling aims to tackle the “grand challenge” of simulating catalytic processes by bridging atomic, molecular, pore, and reactor scales. However, it brings substantial challenges due to the complexity and diversity of phenomena involved, combined by the difficulties in aligning differences in temporal and spatial scales and handling the computational demands across each model layer. Using methane oxidation as a test case a multiscale workflow developed as part of the EU funded ReaxPro project will be presented.

The developed models were validated against experimental data collected through different reactive characterisation techniques. Model predictions demonstrated reasonable agreement with experimental results without any experimental fitting of parameters, highlighting the workflow's potential for tackling the complexities inherent to industrial catalytic processes. The talk will also discuss how newly developed approaches such as MLIPs might fit into such a workflow and be used to accelerate the catalyst discovery process.