Multi-scale Modelling Simulations in Catalytic Material or Process Optimisation

With the advent of high performance computers, it is becoming increasingly interesting to render both the discovery of materials, as well as processing, production or manufacturing digital, let alone that ideally one would be able to link the two in a completely seamless manner. Presentation will contain the cases of atom scale simulations, mesoscale digital workflows, where thermodynamics, kinetics and transport are relevant, as well as large scale systems, where continuum comes into play or techno-economics tell us, which way to pursue. Indeed, this can be explored for some relevant cases, which deal with catalysis, primarily related to chemical energy storage, solar light harvesting, bio-based compound production, the recycling of plastics and many more, some of which will be presented as examples.