CATALYTIC REACTION MECHANISTIC MULTI-SCALE MODELLING SIMULATIONS: LINKING ATOMS–CONTINUUM

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Catalytic reaction mechanistic multi-scale modelling has emerged as a powerful simulation framework for bridging the atomic scale chemistry with industrial continuum level reactor, separator and process behaviour. At electronic, atomistic and molecule modelling levels, first principles calculations, density functional theory and *ab initio* molecular dynamics' simulations provide a fundamental mechanistic insight into surface adsorption energetics, reaction pathways, transition states, structure–activity relationships and selectivity dependence of homogeneous or heterogeneous catalytic materials. These form the basis for micro-kinetics that captures the intrinsic reaction rates/mechanistic selectivity under realistic operating conditions. Beyond isolated active sites, mesoscale accounts for morphology, heterogeneity, and transport. Coupling the micro-kinetics with transport phenomena resistances enables the prediction of the non-isothermal heat effects, mass transfer resistances and chemical concentration gradients across heterogeneous catalyst particles, beds and electrodes. In reactors/processes, models integrate thermodynamics, transport and dynamics to assess performance, efficiency and scalability. Advances demonstrate the integration of the insights into the macroscale for thermo-catalysis, electrochemistry and photo-catalysis, including hydrogen carrier cycles, CO_2 reduction and nitrogen. Such mechanistic, hierarchical and concurrent multi-scale modelling approaches enable rational catalyst design, industrial process optimization and techno-economic technology assessment. Despite progress, challenges remain in efficiency, uncertainty and transferability. A continued computational development of mechanistically consistent multi-scale modelling frameworks is essential for predictive catalysis screening, the accelerated scalable deployment of technologies and digitalisation.

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