catalysts

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(Micro)Kinetics Driven Catalyst and Process Design

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Message from the Guest Editors

Novel catalyst or process design or the optimization of existing ones typically benefits from a fundamental understanding of the mechanisms occurring at a molecular level. An important tool that researchers have in their possession to elucidate these mechanisms is mapping the intrinsic reaction kinetics, and in particular (micro)kinetic model development. Apart from the intrinsic reaction kinetics at the molecular level, transport phenomena at the pellet scale as well as hydrodynamics at the reactor scale may also have to be explicitly accounted for when extrapolating the laboratory kinetics to the industrial scale, resulting in a true multiscale simulation model.

It is within this area, i.e., (micro)kinetics driven catalyst and process design, that contributions to this Special Issue are envisaged. Both experimental studies focusing on the elucidation of intrinsic kinetics aiming at rational catalyst design as well as studies that use (micro)kinetic modeling for this purpose will be considered. Moreover, studies involving multiscale modelling aiming at the design of catalytic processes are warmly welcomed.