

CatLab Lecture Series hosted by FHI and HZB

Friday, February 16th 2024, 10:30-12:00

BESSY II, Seminar Room at the Entrance, Albert-Einstein-Straße 15, Berlin Adlershof

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Multiscale Studies and Engineering of Surface-Reactive Systems

Tomorrow's chemicals are facing massive transitions due to the need for an alternative energy input, changing feedstock, limited resources, varying cost structures, etc. Chemical and reaction engineering is in charge for chemical and electrochemical reactions to meet the upcoming business and technical objectives. For simultaneous process-product design, a multiscale understanding provides opportunities to consider phenomena on different time and length scales of the reaction system.

In this talk, I will show how multiscale studies enable knowledge-based engineering of surface-reactive systems, such as heterogeneous catalytic, electrochemical, and multiphase processes. Examples are presented of catalytic fixed-bed reactors with an emphasis of particle-resolved CFD simulations taking the actual bed structure into account, the coupling with microkinetics, and scale bridging to the plant level. Some of those methods have been transferred successfully to stationary batteries, where pore-scale and cell-scale simulations reveal interactions between transport phenomena and battery performance. Finally, the study of a micro bubble column reactor is discussed showing opportunities and challenges of using multiscale approaches in multiphase systems.