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DATA SCIENCE TOOLS FOR HETEROGENEOUS CATALYST DESIGN

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ETH Hönggerberg, HCI D 2 and on Zoom
(https://ethz.zoom.us/j/61663566631)

Project Summary: Heterogeneous catalysis underpins the development of sustainable chemical technologies, driving the shift toward carbon-neutral chemicals and renewable energy carriers. Advances in tailored synthesis, state-of-the-art characterization, and theoretical modelling, collectively known as the catalyst design toolbox, have enabled the design of heterogeneous catalysts with improved activity, selectivity, stability, and environmental footprint. Yet, unraveling the intricate relationships among synthesis conditions, metal properties, and metal-support interactions, all of which govern nanostructures giving rise to unique material properties, ultimately dictating catalytic performance, remains a significant challenge. To transcend these limitations, data science and machine learning (ML) offer transformative potential. This thesis underscores the systematic and impactful application of data science in advancing heterogeneous catalyst design, focusing on the synthesis-structure-property-performance continuum. Progressing from foundational to complex approaches, the presentation begins by highlighting surrogate modelling and active learning concepts to predict and optimize multimetallic catalyst performance in methanol and higher alcohol synthesis. Then, the potential of explainable ML to uncover structural and electronic properties from kinetic data is illustrated, revealing patterns and catalytic insights not easily discernible by human experts. Lastly, probabilistic ML and language models, along with the critical role of data standardization, are highlighted in the drive towards data-guided synthesis of nanostructured catalysts with experimental reproducibility. These research findings position data-driven modeling as a vital addition to the catalyst design toolbox, offering actionable insights for experimentalists. Integrating data science into experimental workflows propels the vision of digital catalysis, enabling efficient, predictive, and data-informed catalyst design and discovery.

CV: Manu Shivanand Suvarna earned his B.E in Biotechnology from Visvesvaraya Technological University, India (2009) and M.Eng in Chemical and Biological Engineering from the University of British Columbia, Canada (2012). Following eight years of professional experience as a Process Simulation Engineer and Data Scientist in the chemical industry, he commenced his doctoral studies in 2021 in the Advanced Catalysis Engineering group, under the guidance of Prof. Javier Pérez-Ramírez.