ETH zürich

ICB PhD public presentations

NOVEL TOOLS FOR THE DESIGN OF SINGLE-ATOM HETEROGENEOUS CATALYSTS

Dario Faust Akl
ICB/Advanced Catalysis Engineering Group
Supervisor: Prof. Dr. Javier Pérez-Ramírez
Co-examiner: Dr. Sharon Mitchell and
Prof. Dr. Gonzalo Guillén Gosálbez

24/05/2023, 5:00 pm
ETH Hönggerberg, HCI H2.1 and on Zoom
(https://ethz.zoom.us/j/68240909696)

Project Summary: Single-atom heterogeneous catalysts play a pivotal role in the design of new solid catalytic materials with improved metal utilization, novel reactivity patterns, and unparalleled atomic-scale tunability. Despite a decade of development at breakneck speed, pushing the frontiers of synthesis, analytical capabilities, and discovery of new applications were needed to advance the field of SACs. Concepts on how to address the multifaceted challenges in SAC design developed in this thesis will be showcased. A scalable and automatable two-step preparation method enables the synthesis of SACs with distinct metal contents and surface atomic densities, allowing the assessment of ultra-high-density SACs in two prototypic applications. To estimate statistically robust metrics for single atom proximity in SACs from electron microscopy images, a generalizable, AI-driven atom-detection tool was developed. Three separate case studies illustrate diverse aspects of SAC design, such as (i) precursor nuclearity effects in iron hydrogenation catalysts, (ii) the environmental impact assessment of reusable palladium catalysts for the Sonogashira coupling reaction, and (iii) the *in situ* formation of copper active species in acetylene hydrochlorination. The presented findings illustrate potential design strategies for improved and more sustainable SACs.

CV: D. Faust Akl pursued a B.Sc. in Chemical Engineering at the Technical University of Berlin (2017) followed by an M.Sc. at ETH Zurich (2019). He conducted his doctoral studies within the SNSF-funded NCCR Catalysis in the advanced Catalysis engineering group led by Prof. J. Pérez-Ramírez, co-supervised by Dr. S. Mitchell.