

ICB PhD public presentations**TOWARD SUSTAINABLE CROSS-
COUPLINGS THROUGH THE DESIGN
OF HETEROGENEOUS Pd SINGLE-
ATOM CATALYTIC SYSTEMS****Dario Poier**

ICB/Advanced Catalysis Engineering Group

Supervisor: Prof. Dr. Javier Pérez-Ramírez

Co-examiner: Prof. Dr. Roger Marti, Dr. Sharon Mitchell and
Prof. Dr. Ali Çoskun**27/09/2024, 2:00 pm****ETH Hönggerberg, HCI D 2 and on Zoom****(<https://ethz.zoom.us/j/63577064529>)**

Project Summary: Transition metal catalysis presents an irreplaceable tool for the fine chemical industry. Yet, the high cost and environmental footprint of precious metals commonly applied and difficulties in their post-use recovery have prompted the search for solid-supported alternatives to broadly employed organometallic complexes. Through the example of Sonogashira-Hagihara coupling, this thesis shows that heterogeneous single-atom catalysts (SAC) offer a promising opportunity to improve the sustainability of cross-couplings. Their use will be motivated by showcasing the environmental benefits of their recyclability, before establishing criteria for choosing a catalytic system. Subsequently, the influence of the reaction environment on the performance of a palladium SAC will be addressed, setting the basis for demonstrating the multigram synthesis of an Erlotinib anti-cancer drug intermediate under optimized conditions. Lastly, to understand the role of phosphine ligands in the activation of SACs and assess their potential for tailoring the 3D environment of the metal sites, a common strategy in homogeneous catalysis, the effect of their geometric and electronic properties on the catalytic activity of the Pd-SAC is elucidated. The findings emphasize the need to understand the interactions between SACs and the reaction environment to harness the catalyst's full potential and illustrate design strategies for SAC systems in cross-coupling reactions.

CV: Dario Poier obtained an MSc in Chemistry from Bielefeld University (2020) before starting his doctoral research in a collaborative project funded by NCCR Catalysis and jointly supervised by Prof. Javier Pérez-Ramírez and Prof. Roger Marti.