

ICB PhD public presentations**CARBON NITRIDE AS A PLATFORM FOR SINGLE METAL ATOMS AND LOW-NUCLEARITY CLUSTERS****Evgeniya Vorobyeva**

ICB/Advanced Catalysis Engineering Group

Supervisor: Prof. Dr. Javier Pérez-Ramírez

Co-examiner: Prof. Dr. Chih-Jen Shih

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Project Summary: Single-atom heterogeneous catalysts (SAHCs) receive considerable attention due to the potential for every atom to contribute to catalytic turnover in a targeted application, but also displaying many individual characteristics compared to bulk metals. The first stable SAHC exploited the N-rich scaffold of carbon nitrides (CN). This thesis explores the scope of SAHCs based on CN for various chemical transformations, combining state-of-the-art experiments and theory to interpret the observed behavior. Extrapolation to distinct metals, reveals the importance of optimizing the synthetic approach and of exposing the metal sites at the surface. The strength of the metal-carrier interaction, which can be tuned by varying the chemical composition and crystal structure of the host, is an important parameter to maximize the activity of Pd-SAHCs in the semi-hydrogenation of alkynes. The strong resemblance of metal centers in SAHCs to those in organometallic complexes prompted their exploration in homogeneously catalyzed Suzuki coupling and amine arylation reactions, highlighting exciting prospects for the heterogenization of challenging organic processes. Extending to low-atomicity metal species, the ability of CN to accommodate dimers and trimers was used to resolve the nuclearity effects on the catalytic performance, revealing opposite trends in distinct applications. The results identify key design criteria for the development of atom-efficient catalysts and highlight current limitations in the study of these advanced materials.

CV. E. Vorobyeva obtained her Specialist Degree in Physical Chemistry at Lomonosov Moscow State University in 2015. The same year, she joined the group of Prof. Dr. J. Pérez-Ramírez for her doctoral studies.