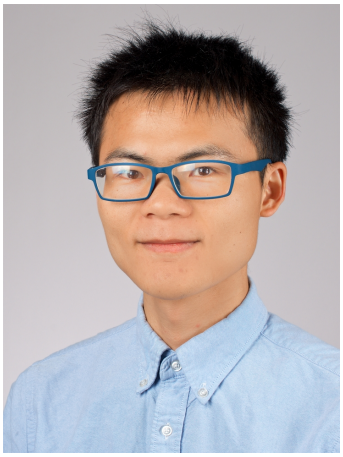
ETH zürich

ICB PhD public presentations

THERMODYNAMIC BEHAVIOR OF SUPPORTED TRANSITION-METAL BASED HETERO-GENEOUS CATALYSTS



Xing Wang

The van Bokhoven Group
Supervisor: Prof. Dr. Jeroen Anton van Bokhoven
Co-examiners: Prof. Dr. Christophe Copéret and Dr. Dennis Palagin

ETH Hönggerberg, 11/02/2020
HCI D 8, 10.00 h

Project Summary: Transition-metal nanoparticles on oxide supports are known as one of the most important classes of heterogeneous catalysts and are widely used in chemical transformations, environmental pollution control and sustainable energy systems. My PhD research focuses on the computational understanding of the thermodynamic behavior of atomically dispersed platinum catalysts on oxide supports, as well as the interaction between titania monolayer and transition-metal particles, by using density functional theory calculations and ab initio atomistic thermodynamics modeling. We demonstrate that atomically dispersed platinum species on ceria can adopt a range of local coordination configurations and oxidation states that depend on the environmental conditions. Encapsulation of transition-metal by a reduced titania overlayer, also known as the classical strong metal–support interaction (SMSI), was predicted by thermodynamic driving force analysis. Our theoretical modeling provide an atomic insight into the sintering and redispersion of nanoparticles, as well as into the SMSI under realistic conditions.

CV: Xing received his BSc and MSc in Materials Science and Engineering from Central South University, China. In April 2016, he started his doctoral studies in the group of Prof. van Bokhoven.