Bio

The focus of my research is implementation of advanced methods to gain structural information from X-ray absorption spectra of heterogeneous catalysts under operating conditions. Structural dynamics can be very subtle and chemical structures yet unknown. By applying high-sensitivity detection methods (e.g., HERFD-XAS*) and theoretically calculating spectra of hypothetical structures, I enhance the sensitivity of conventional techniques and create shortcuts to new discoveries. Particular systems of interest are single-site catalysts, serving as excellent models for examining reaction mechanisms and intermediate species on well-defined sites. Furthermore, I study activation and de-activation of catalysts for globally important energy-related processes.

Expertise

• Experimental X-ray absorption spectroscopy: sample optimization, data acquisition and analysis
• In situ cell design
• Molecular models for EXAFS refinement
• XANES and L-DOS calculations using FEFF9

*High-energy-resolution fluorescence-detected X-ray absorption spectroscopy, a method with monochromatic fluorescence detection, unlike energy-dispersive fluorescence detection with a much lower energy resolution.

PROFESSIONAL EDUCATION

• Ph. D., Karlsruhe Institute of Technology, Chemical Technology (2014)
• Master of Science, University of Copenhagen, Nanoscience (2009)
• Bachelor of Science, University of Copenhagen, Nanotechnology (2007)

Publications

PUBLICATIONS

• Structural evolution of atomically dispersed Pt catalysts dictates reactivity. Nature materials

• Role of Co2C in ZnO-promoted Co Catalysts for Alcohol Synthesis from Syngas CHEMCATCHEM
• Synthesis of Colloidal Pd/Au Dilute Alloy Nanocrystals and Their Potential for Selective Catalytic Oxidations. Journal of the American Chemical Society
  Wrasman, C. J., Boubnov, A., Riscoe, A. R., Hoffman, A. S., Bare, S. R., Cargnello, M.
  2018

• Synergistic effect in colloidal Pd/Au single atom alloy nanocrystals for selective oxidations
  Wrasman, C., Riscoe, A., Hoffman, A., Boubnov, A., Bare, S., Cargnello, M.
  AMER CHEMICAL SOC.2018

• Biomimetic oxidation catalyst from polymer-nanocrystal composite material
  Riscoe, A., Wrasman, C., Hoffman, A., Menon, A., Boubnov, A., Goodman, E., Bare, S., Cargnello, M.
  AMER CHEMICAL SOC.2018

• Low-Temperature Restructuring of CeO2-Supported Ru Nanoparticles Determines Selectivity in CO2 Catalytic Reduction. Journal of the American Chemical Society
  2018; 140 (42): 13736–45