

Segregation Phenomena in Size-Selected Bimetallic CuNi Nanoparticle Catalysts for CO₂ hydrogenation

Ioannis Zegkinoglou¹, Lukas Pielsticker¹, Nuria J. Divins¹, Beatriz Roldán Cuenya^{1,2}

¹Department of Physics, Ruhr University Bochum, 44780 Bochum, Germany

²Department of Interface Science, Fritz-Haber Institute of the Max Planck Society, Berlin 14195, Germany

Ioannis.Zegkinoglou@rub.de

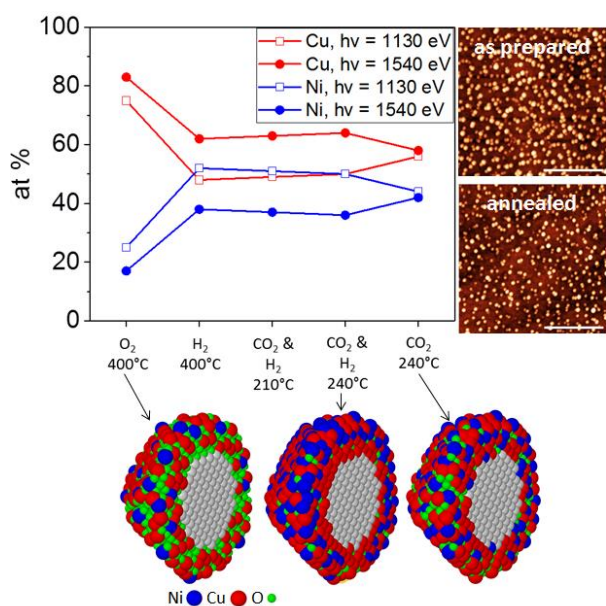


Figure 1: Cu (red) and Ni (blue) atomic percentages of CuNi nanoparticles as determined *in situ* with NAP-XPS upon annealing in various gases. AFM images of the nanoparticles before and after annealing and atomic models illustrating their elemental composition are also shown.

Catalytic systems based on bimetallic alloy nanoparticles (NPs) often exhibit significantly superior catalytic properties compared to their monometallic counterparts. The spatial atomic distribution and chemical state of the two metals play a pivotal role in the efficiency and stability of the catalysts. Employing near-ambient pressure (NAP-XPS) and ultrahigh vacuum X-ray photoelectron spectroscopy (XPS) together with atomic force microscopy (AFM), we systematically investigated surface segregation, restructuring, and sintering phenomena in size-controlled copper-nickel nanoparticles supported on silicon substrates as a function of temperature, chemical state, and reactive gas environment [1]. The depth profile of the elemental composition of the particles was determined under operando CO₂ hydrogenation conditions by varying the X-ray photon energy. The changes in the morphology induced by adding CO to the reaction mixture were also investigated. Our study showed that the initial chemical state of the NPs and the adsorbate-induced effects sensitively affect restructuring and surface segregation in CuNi nanocatalysts,

suggesting that their catalytic properties can be tuned by appropriate plasma and annealing treatments prior to the reaction as well as by control of the reaction mixture composition.

References:

[1] L. Pielsticker, I. Zegkinoglou, N. J. Divins, H. Mistry, Y.-T. Chen, A. Kostka, J. A. Boscoboinik, B. Roldan Cuenya, *J. Phys. Chem. B* **122**, 919 (2018).