Structure Sensitivity in Heterogeneous Catalysis – Prof. dr. Emiel J.M. Hensen

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Short biography

2009 – present	Professor of Inorganic Materials Chemistry & Head of laboratory; TU/e
2008 – 2009	Associate Professor; Department of Chemical Engineering; TU/e
2006 – 2008	Part-time researcher; Shell Research and Technology Center Amsterdam
2002 – present	Part-time lecturer; Katholieke Universiteit Leuven
2002 – 2007	Assistant Professor; Department of Chemical Engineering; TU/e
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Abstract

Catalysis is the science and technology of the control of the change in the molecular structure of reactants to products ("chemical reaction") by functional materials ("the catalyst"). Not only does a good catalyst accelerate the chemical reaction, it also determines the direction of chemical transformation on the energy landscape and therefore selectivity. The development of certain overlayers on the surface may lead to catalyst deactivation and thus limit catalyst stability. One of the great challenges to heterogeneous catalysis is to understand the dependence of the activity, selectivity and stability of catalytic reactions on particle size and shape. The nanoscale dimensions of metal particles in catalysts result in a very high reactive surface area. The intriguing aspect of nanoparticle catalysis is that unique behavior appears when they become smaller than 10 nm. In this regime their surface contains a significant fraction of surface atoms with a lower coordination number (corners and edges) than terrace atoms, exhibiting a dramatically different activity and selectivity. On nanoparticles the surface atoms may also form unique topologies, e.g. step-edge sites, which affect catalytic behavior.

In the lecture, modern insights about structure sensitivity in heterogeneous catalysis will be highlighted using several case studies on methane steam reforming, the Fischer-Tropsch reaction and carbon monoxide oxidation on ceria-supported metal nanoparticles. The work explores the use of kinetic studies and novel methods to characterize metal nanoparticle surfaces for heterogeneous model systems. Quantum-chemical studies of elementary reaction steps on relevant model surfaces are used to determine kinetic parameters which are used as input for microkinetic simulations to predict macroscopic activity and selectivity.