



Closing Symposium of the Collaborative Research Centre SFB 558
 "Metal-substrate interactions in heterogeneous catalysis": 2000-2012

Conference Hall of the RUB (Veranstaltungszentrum der RUB) April 16-18, 2012

**"Metal-support interactions –
 How important are they in heterogeneous catalysis, electro- and photo-catalysis?"**

Monday April 16, 2012	
13.00 – 13.40	REGISTRATION
13.40 – 13.50	WELCOME by Prof. Dr. E. Weiler , Rector of the Ruhr-Universität Bochum
13.50 – 14.00	WELCOME by Prof. Dr. D. Marx , Dean of the Faculty of Chemistry and Biochemistry
14.00 – 14.10	WELCOME by Prof. Dr. M. Muhler , Speaker of the SFB 558
14.10 – 15.10	Robert Schlögl, FHI, Berlin Functional analysis of the Cu/ZnO system
15.10 – 16.10	Philippe Sautet, University of Lyon CNRS and Ecole Normale Supérieure of Lyon, Lyon, France Metal-Substrate-Interactions: what can we learn from computational chemistry ?
16.10 – 16.40	COFFEE BREAK
16.40 – 17.20	Christof Wöll, KIT, Karlsruhe The Surface Science Approach for Understanding Reactions on Oxide Powders: The Importance of IR Spectroscopy
17.20 – 18.00	Dominik Marx, Theoretische Chemie, RUB Heterogeneous Catalysis from Molecular Dynamics
18.00 – 18.40	Jan-Dierk Grunwaldt, KIT, Karlsruhe Shining light on catalysts at work: From the micro to the nanoscale
	RECEPTION and POSTER SESSION



Tuesday April 17, 2012	
09.00 – 09.40	Roland Fischer, Anorganische Chemie II, RUB Perspectives of Metal-Organic Frameworks for Catalysis
09.40 – 10.20	Martin Muhler, Technische Chemie, RUB Probing metal-support interactions in ZnO-based catalysts: from bulk materials to supported catalysts and colloids
10.20 – 10.50	COFFEE BREAK
10.50 – 11.20	Wolfgang Grünert, Technische Chemie, RUB Metal-support interactions studied with model systems encapsulated in mesopores – challenges and insights
11.20 – 12.00	Jürgen Behm, Universität Ulm Metal-support interactions in supported Au catalyst
12.00 – 13.20	LUNCH BREAK
13.20 – 14.00	Karina Morgenstern, Physikalische Chemie I, RUB Interaction of NaCl with a metal support and its influence on molecular switches
14.00 – 14.40	Martin Stratmann, MPI für Eisenforschung, Düsseldorf Electrocatalysis: How to answer major questions in fundamental research
14.40 – 15.20	Alfred Ludwig, Inst. für Werkstoffe, RUB Development of Functional Materials using High-Throughput Thin Film Experimentation
15.20 – 15.50	COFFEE BREAK
15.50 – 16.30	Guido Mul, Universität Twente, NL How Au affects TiO ₂ based photocatalysis
16.30 – 17.00	Klaus Merz, Anorganische Chemie I, RUB Oxidation of 2-propanol over Gold and Palladium catalysts
17.00 – 17.30	Yuemin Wang, Technische Chemie, RUB Structural and electronic properties of defects on/in oxides studied by vibrational spectroscopy
17.30 – 18.00	Michael Wark, Technische Chemie, RUB Mixed metal oxide photocatalysts for hydrogen production by visible light induced water splitting
	DINNER at Henrichs, Hattingen

Wednesday April 18, 2012

09.00 – 09.40	Ferdi Schüth, MPI für Kohlenforschung, Mülheim Interaction between Gold and Support Material in Highly Active Gold Catalysts
09.40 – 10.10	André van Veen, Technische Universität München Probing of metal-substrate interactions by transient kinetic methods
10.10 – 10.40	Anja-Verena Mudring, Anorganische Chemie I, RUB Nanomaterials for Catalysis from Ionic Liquids
10.40 – 11.10	COFFEE BREAK
11.10 – 11.50	Ralf Drautz, ICAMS, RUB Simplified models of the electronic structure for predicting phase stability
11.50 – 12.30	Bernd Meyer, ICMM/CCC, Universität Erlangen-Nürnberg Reduction versus Protonation of Oxide Surfaces: From the Gas Phase to the Liquid
12.30 – 14.00	LUNCH BREAK
14.00 – 14.30	Jörg Behler, Theoretische Chemie, RUB Neural Network Potentials for Large-Scale Simulations of Copper and Zinc Oxide
14.30 – 15.00	Rochus Schmid, Anorganische Chemie II, RUB First principles derived force fields to understand structure and dynamics of metal-organic frameworks
15.00 – 15.30	COFFEE BREAK
15.30 – 16.00	Christof Hättig, Theoretische Chemie, RUB Embedded cluster calculations on the methanol synthesis on ZnO(000-1) and defects in the ZnO bulk
16.00 – 16.30	Ulrich Köhler, Experimentalphysik, RUB The Thermal Interaction of Copper with Zinc Oxide
16.30 – 17.00	Alexander Birkner, Physikalische Chemie I, RUB Oxidation behavior of orientated brass surfaces
17.00 – 17.30	CLOSING REMARKS