



XV. International Symposium on Relations between Homogeneous and Heterogeneous Catalysis

Berlin, September 11 - 16, 2011

Scientific Programm





XV. International Symposium on Relations between Homogeneous and Heterogeneous Catalysis, Berlin, September 11 - 16, 2011

Sun

Registration

Sunday, Sept. 11, 2011

17:00	-	21:00	Registration
19:00	-	22:00	Welcome Reception
			Conference Centre Harnack House Ihnestraße 16-20, 14195 Berlin http://www.harnackhaus-berlin.mpg.de/eng-index.htm

Mon

Registration

Monday, Sept. 12, 2011

08:30			Registration Henry Ford Building of Freie Universität Berlin, Garystraße 35, 14195 Berlin (Entrance also from the Boltzmannstraße) http://www.fu-berlin.de/en/sites/hfb/anfahrt/index.html
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Monday, Sept. 12, 2011, Audi Max

09:00	-	09:10	Hajo Freund: Opening remarks
09:10	-	09:30	Matthias Driess: Presentation of the Cluster of Excellence "Unifying Concepts in Catalysis" (UniCat)
1. Session, Session Chair: Hajo Freund			
09:30	-	10:15	Plenary Speaker Heterogeneous Catalysis: Kazunari Domen <i>Water splitting into hydrogen and oxygen on heterogeneous photocatalysts</i>
10:15	-	11:00	Plenary Speaker Biocatalysis: Itamar Willner <i>Programmed Catalysis with DNA Nanostructures and Hybrid Systems</i>
11:00	-	11:30	coffee
2. Session, Session Chair: Cynthia Friend			
11:30	-	12:15	Plenary Speaker Heterogeneous/Homogeneous Catalysis: Peter Wasserscheid <i>Catalytic Technologies Involving Supported Ionic Liquid Films</i>
12:15	-	12:50	Keynote Speaker Homogeneous Catalysis: Jan-E. Bäckvall <i>Biomimetic Catalysis in Green Organic Transformations</i>
12:55	-	14:30	lunch
3. Session, Session Chair: Siegfried Blechert			
14:30	-	15:05	Keynote Speaker Homogeneous Catalysis: Ronny Neumann <i>Polyoxometalates as Oxidation Catalysts: Electron Transfer-Oxygen Transfer Reactions in Solution and Insights into the Mars-Van Krevelen Mechanism</i>
15:05	-	15:40	Keynote Speaker Heterogeneous Catalysis: Can Li <i>Homogeneous Chiral Catalysis in Heterogeneous Nanoreactors</i>
15:40	-	16:10	coffee





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4. Session, Session Chair: Jan-Erlin Bäckvall

16:10 - 16:45	Keynote Speaker Homogeneous Catalysis: Roy Periana <i>Design and Study of new Homogeneous Catalysts for Small Molecule Activation and Conversion</i>
Session Homogeneous Catalysis:	
16:45 - 17:05	Maria-José Calhorda <i>The role of oxo and peroxo Mo(VI) complexes in oxidation processes</i>
17:05 - 17:25	Dieter Vogt <i>Continuous Homogeneous Catalysis Applying Nanofiltration: Hydroformylation with MWE Catalysts</i>





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Monday, Sept. 12, 2011, Lecture Hall A

Lecture Hall A	5. Session, Session Chair: Micha Asscher
(parallel):	
	Session Heterogeneous Catalysis:
12:15 - 12:35	Kamel Ait-Mansour <i>Influence of the reduction state of TiO₂(110) on the catalytic CO oxidation on supported Pt nanoclusters</i>
12:35 - 12:55	Ulla Simon <i>Stabilization of Li in MgO due to cation codoping</i>
12:55 - 14:30	lunch
	6. Session, Session Chair: Silvia Bordiga
14:30 - 14:50	Kazuhiko Amakawa <i>Origin of active sites for propene metathesis in MoOx/SBA-15</i>
14:50 - 15:10	Xiao Xie <i>Synthesis of porous NiMnO and application in dry reforming of methane</i>
15:10 - 15:30	Kenji Wada <i>Development of Solid Ru/CeO₂ Catalysts for the Addition of Carboxylic Acids to Terminal Alkynes</i>
15:40 - 16:10	coffee
Lecture Hall A	7. Session, Session Chair: Graham Hutchings
	Session Homogeneous Catalysis:
16:10 - 16:30	Katrin Driller <i>A General and Selective Iron-catalyzed Aminocarbonylation of Alkynes: Synthesis of Acryl- and Cinnamides and Succinimide</i>
16:30 - 16:50	Stephan Enthaler <i>Zinc Chemistry – From a “Boring” Element to Fascinating Applications in Catalysis</i>
16:50 - 17:10	Lele Duan <i>Fast mononuclear Ru water oxidation catalysts: catching up the activity of oxygen evolving complex in PSII</i>





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Tuesday, Sept. 13, 2011, Audi Max

8. Session, Session Chair: Kazunari Domen	
09:00 - 09:45	Plenary Speaker Heterogeneous Catalysis: Avelino Corma <i>Single isolated sites in solid catalysts for bridging the gap with homogeneous catalysts</i>
09:45 - 10:30	Plenary Speaker Biocatalysis: Donald Hilvert <i>Designer Enzymes</i>
10:30 - 11:15	Plenary Speaker Heterogeneous Catalysis: Graham Hutchings <i>Catalysis using gold and gold palladium nanoparticles</i>
11:15 - 11:45	coffee
9. Session, Session Chair: Joachim Sauer	
11:45 - 12:20	Keynote Speaker Heterogeneous Catalysis: Robert Schlögl <i>Active sites in heterogeneous catalysis</i>
12:20 - 12:55	Keynote Speaker Theory: Odile Eisenstein <i>Determining reaction mechanisms: the input from computational chemistry</i>
12:55 - 14:30	lunch
10. Session, Session Chair: Christian Limberg	
14:30 - 15:05	Keynote Speaker Homogeneous Catalysis: Shannon Stahl <i>Aerobic Oxidation of C-H Bonds Catalyzed by Palladium</i>
15:05 - 15:40	Keynote Speaker Heterogeneous Catalysis: Unni Olsbye <i>Conversion of methanol to hydrocarbons - how the zeolitic host structure affects product selectivity</i>
15:40 - 16:10	coffee





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Tuesday, Sept. 13, 2011, Audi Max

13. Session, Session Chair: Matthias Driess

Session Biocatalysis:

16:10	-	16:30	Wolfgang Kroutil <i>Biocatalytic oxidative enantioselective C-C-formation as the key step in the chemoenzymatic synthesis of novel optically pure berbine alkaloids</i>
16:45	-	17:05	Ingo Zebger <i>Learning from biological hydrogen catalysis: spectroscopic studies on structure and function of oxygen tolerant and anaerobic [NiFe]-hydrogenases</i>
17:05	-	17:25	Michael Fuchs <i>Chem-Enzymatic Cascade Reactions Based on Galactose Oxidase</i>





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Tuesday, Sept. 13, 2011, Lecture Hall A

Lecture Hall A	11. Session, Session Chair: Amy Rosenzweig
	Session Homogeneous Catalysis:
11:45 - 12:05	Yurii Geletii <i>Immobilization of polyoxometalate based water oxidation catalysts on anodes. Water electrolysis using modified anodes</i>
12:05 - 12:25	Kallol Ray <i>O-O bond formation mediated by a hexanuclear iron complex supported on a stannoxane core</i>
12:25 - 12:45	Giuliano Giambastiani <i>Facing Unexpected Reactivity Paths with Group-IV Amido-Pyridinate Polymerization Catalysts</i>
12:55 - 14:30	lunch
Lecture Hall A	12. Session, Session Chair: Robert Bittl
	Session Biocatalysis:
14:30 - 14:50	Lars Lauterbach <i>A modular approach to understand the catalytic sub-reactions of the NAD⁺-reducing [NiFe]-hydrogenase from <i>Ralstonia eutropha</i></i>
14:50 - 15:10	Niklas Meine <i>From cellulose to water-soluble products: the role of mechanocatalysis</i>
	Session Heterogeneous Catalysis:
15:10 - 15:30	Elin Larsson <i>Operando Catalyst Sintering and Activity Measurements Using Indirect Nanoplasmonic Sensing</i>
15:40 - 16:10	coffee
Lecture Hall A	14. Session, Session Chair: Uni Olsbye
16:10 - 16:30	Kazuya Yamaguchi <i>Aerobic Oxidative Transformation of Azides to Nitriles by Supported Ruthenium Hydroxide Catalyst</i>
16:30 - 16:50	Ivelina Zaharieva <i>Electrosynthesis, functional and structural characterization of a water-oxidizing manganese oxide</i>
16:50 - 17:10	Hiroyuki Yamaura <i>Investigation on reduction behavior of CuO-loaded SnO₂ by simultaneous measurements of TPR and electric resistance</i>
Foyer:	
18:00 -	Poster Session I





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Wednesday, Sept. 14, 2011, Audi Max

15. Session, Session Chair: Avelino Corma	
09:00 - 09:45	Plenary Speaker Heterogeneous Catalysis: Fraser Armstrong <i>Efficient Electrocatalysts for Future Energy Technology: The Importance of Understanding How Enzymes Work so Well</i>
09:45 - 10:30	Plenary Speaker Theory: Joachim Sauer <i>Catalytically active metal oxides in different environments. Quantum chemical approach</i>
10:30 - 11:15	Plenary Speaker Heterogeneous Catalysis: Cynthia Friend <i>Insights into Heterogeneous Catalytic Processes from Fundamental Surface Chemistry: A Molecular View</i>
11:15 - 11:45	coffee
16. Session, Session Chair: Itamar Willner	
11:45 - 12:20	Keynote Speaker Homogeneous Catalysis: Siegfried Blechert <i>Stereocontrolled Olefin Metathesis</i>
12:20 - 12:55	Keynote Speaker Heterogeneous Catalysis: Silvia Bordiga <i>NO adsorption on transition metal ions in microporous materials followed by combined use of spectroscopies</i>
13:00	Conference Photo at the Harnack House
13:15	lunch
14:00 - 16:00	Walking Tour: Berlin Highlights and the sky over Berlin
19:00 - 23:00	Conference Dinner





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Wed

Scientific Program

Wednesday, Sept. 14, 2011, Lecture Hall A

		17. Session, Session Chair: Wataru Ueda
Lecture Hall A (parallel):		Session Heterogeneous Catalysis:
11:45 -	12:05	Hynek Balcar <i>Grubbs and Hoveyda-Grubbs olefin metathesis catalysts immobilized on mesoporous molecular sieves</i>
12:05 -	12:25	Elena Groppo <i>Spectroscopic investigation of heterogeneous Ziegler-Natta catalysts: Ti and Mg chloride tetrahydrofuranates, their interaction compound and the role of the activator</i>
12:25 -	12:45	Satoshi Muratsugu <i>Preparation and Selective Catalytic Behavior of Molecularly Imprinted Ru Catalysts on a SiO₂ Surface Acting in Water Media</i>
13:00		Conference Photo at the Harnack House
13:15		lunch
14:00 -	16:00	Walking Tour: Berlin Highlights and the sky over Berlin
19:00 -	23:00	Conference Dinner





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Thursday, Sept. 15, 2011, Audi Max

		18. Session, Session Chair: Peter Wasserscheid
09:00	- 09:45	Plenary Speaker Biocatalysis: Amy Rosenzweig <i>Biological methane oxidation</i>
09:45	- 10:30	Plenary Speaker Homogeneous Catalysis: John F. Hartwig <i>Catalytic Transformations of Arenes</i>
10:30	- 11:05	Keynote Speaker Homogeneous Catalysis: Tobin Marks <i>Oxide Surfaces as Activators and Ligands for Organometallic Molecule-Derived Catalysts</i>
11:10	- 11:40	coffee
		20. Session, Session Chair: Klaus Hermann
11:40	- 12:15	Keynote Speaker Heterogeneous Catalysis: Wataru Ueda <i>Complex metal oxide catalysts with high-dimensional crystal structure as well as molecularity</i>
		Session Homogeneous Catalysis:
12:15	- 12:35	Ronald Lindner <i>Investigation of Fundamental Steps in the Formation of Acrylates from CO₂ and Ethylene</i>
12:40	- 14:30	lunch
		22. Session, Session Chair: Stephen Hashmi
14:30	- 14:50	Bhisma Patel <i>Copper (I)-Catalyzed Cascade Synthesis of Bioactive Heterocycles</i>
14:50	- 15:10	Andrea Rossin <i>Ammonia borane dehydrogenation by Iridium and Palladium organometallics</i>
15:10	- 15:30	Hidehiro Sakurai <i>Bimetallic Gold/Palladium Nanoclusters Catalyze the Suzuki-Miyaura Cross-Coupling of Chloroarenes at Room Temperature</i>
15:30	- 16:00	coffee





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Thursday, Sept. 15, 2011, Audi Max

23. Session, Session Chair: Elsie Alessandra Quadrelli	
16:00 - 16:20	Charles Vriamont <i>π-π stacking for immobilization of homogeneous catalyst onto nanotubes: application to MWNTs- supported gold complexes</i>
16:20 - 16:40	Nanna Ahlsten <i>Ir-Catalysed Formation of C-F Bonds: From Allylic Alcohols to α-Fluoroketones</i>
16:40 - 17:00	A. Stephen K. Hashmi <i>On Support Synthesis of Carbene Complexes</i>
18:00 - 20:00	Poster Session II





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Thursday, Sept. 15, 2011, Lecture Hall A

Lecture Hall A	19. Session, Session Chair: Ilme Schlichting
(parallel):	
	Session Heterogeneous Catalysis:
10:30 - 10:50	Elsje Alessandra Quadrelli <i>Hydrodesulfurisation catalyst obtained by Mo(CO)₆ grafting on the MOF Ni₂(dhtp) (h4dhtp = 2,5-dihydroxyterephthalic acid)</i>
10:50 - 11:10	Roberto Rinaldi <i>The role of solvent in the hydrogenolysis of lignin over Ni-catalysts</i>
11:10 - 11:40	coffee
	21. Session, Session Chair: Mizuki Tada
11:40 - 12:00	Kristofer Eriksson <i>Immobilization and Performance of a Biomimetic Oxidation Catalyst on Silica Particles</i>
12:00 - 12:20	José Fraile <i>Enantioselective C-H carbene insertions with homogeneous and immobilized copper complexes</i>
12:20 - 12:40	Koteswara Rao Vuyyuru <i>Conversion of Cellulosic Biomass: A Perspective of Heterogeneous Catalysis</i>
12:40 - 14:30	lunch
Lecture Hall A	24. Session, Session Chair: Sergey Levchenko
	Session Theory:
14:30 - 14:50	Beverly Stewart <i>Computational evidence for facile creation of active 16e- Ru-complexes via a CO-dissociation pathway</i>
14:50 - 15:10	Claudio Greco <i>Redox and electronic properties of the entire iron-sulfur cluster chain in [FeFe]-hydrogenases: a QM/MM investigation</i>
15:10 - 15:30	Marcela Beltran Sanchez <i>Theory and PES Experiments on Rh_nCo_m Cluster</i>
15:30 - 16:00	coffee





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Thursday, Sept. 15, 2011, Lecture Hall A

Lecture Hall A	25. Session, Session Chair: Elena Groppo
	Session Heterogeneous Catalysis:
16:00 - 16:20	Arne Thomas <i>Bridging homogeneous and heterogeneous catalysis by polymerizing molecular catalysts</i>
16:20 - 16:40	Marco Ranocchiari <i>Fast and High Yielding Post-Synthetic Modification of Metal-Organic Frameworks by Vapor Diffusion</i>
16:40 - 17:00	Elad Gross <i>Diastereoselective Heterogeneous Au Nanoparticle catalyst for Homogeneous Olefin Cyclopropanation Reaction in Solution</i>
18:00 - 20:00	Poster Session II





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Friday, Sept. 16, 2011, Audi Max

26. Session, Session Chair: Tobin Marks	
09:00 - 09:45	Plenary Speaker Biocatalysis: Ilme Schlichting <i>Flavin-based photoreceptors - from structure to mechanism to application</i>
09:45 - 10:30	Plenary Speaker Homogeneous Catalysis: William D. Jones <i>Strong C-H and C-C Bond Cleavage Reactions using Homogeneous Transition Metal Complexes</i>
10:30 - 11:05	Keynote Speaker Homogeneous Catalysis: Justin Notestein <i>Supported oxide cluster and oxide cavity catalysts inspired by biology</i>
11:10 - 11:40	coffee
28. Session, Session Chair: Fraser Armstrong	
11:40 - 12:15	Keynote Speaker Theory: Kazunari Yoshizawa <i>Computational Mutation on the Structure and Reactivity of Enzymes</i>
12:15 - 12:50	Keynote Speaker Heterogeneous Catalysis: Mizuki Tada <i>Time/space-resolved XAFS characterization of heterogeneous catalysts</i>
12:50 - 14:30	lunch
30. Session, Session Chair: William D Jones	
Session Homogeneous Catalysis:	
14:30 - 14:50	Mario Simoes <i>Biomimetic oxidation of organic compounds</i>
14:50 - 15:10	Peter Roesky <i>Rare Earth Metal Amido Complexes as Catalyst for the Hydroamination / Cyclization, Hydrosilylation, and Sequential Hydroamination / Hydrosilylation Reaction</i>
15:10 - 15:30	Vital Yazerski <i>Dendritic S,S-TsDPEN Ligands for Iron-catalyzed Asymmetric Olefin Epoxidation</i>
15:30 - 16:00	coffee





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Friday, Sept. 16, 2011, Audi Max

32. Session, Session Chair: Hajo Freund

Session Heterogeneous Catalysis:

16:00 - 16:20	Micha Asscher <i>The role of reduced oxide sites on the stability, morphology, reactivity and selectivity of supported bimetallic clusters</i>
16:20 - 16:50	Poster Award Ceremony
16:50	Concluding Remarks





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Friday, Sept. 16, 2011, Lecture Hall A

Lecture Hall A (parallel): 27. Session, Session Chair:	
Session Heterogeneous Catalysis:	
10:30 - 10:50	Nicholas Brunelli <i>Bifunctional Materials for Cooperative Catalysis through Incorporation of Brønsted Acid and Lewis Base Components</i>
10:50 - 11:10	Jackson Scholten <i>Metal Nanoparticles in Ionic Liquids: Selective Catalysts and Evidences of Nanoparticle/Ionic Liquid Interaction by Isotope Exchange</i>
11:10 - 11:40	coffee
29. Session, Session Chair: Can Li	
11:40 - 12:00	Chloé Thieuleux <i>Preparation of monometallic or plurimetallc nanoparticles (M = Pt, Au, Pt₃Sn) via a colloidal approach: Application as homogeneous nano-catalysts and as heterogeneous catalysts when selectively incorporated in the pores or in walls of mesostructured silica matrices</i>
12:00 - 12:20	Vahideh Habibpour <i>Heterogeneous catalysis by novel size-selected nanocluster powders under realistic reaction conditions</i>
12:20 - 12:40	Swetlana Schauer mann <i>Heats of adsorption and surface reaction for CO and O on Pd nanoparticles as determined by UHV single crystal microcalorimetry</i>
12:40 - 14:30	lunch
Lecture Hall A (parallel): 31. Session, Session Chair: Swetlana Schauer mann	
Session Theory:	
14:30 - 14:50	Peter Saal frank <i>The role of electron-hole pairs for molecular dynamics at surfaces</i>
14:50 - 15:10	Dorota Rutkowska-Zbik <i>DFT Studies on Catalytic Activity of Manganese Porphyrins</i>
15:10 - 15:30	Sergey Levchenko <i>Electronic structure and stoichiometry of Li-MgO and Fe-MgO surfaces at realistic conditions: A theoretical study</i>
15:30 - 16:00	coffee

