

SCIENTIFIC AND METHOD MODULES

Module name	Minisymposium Smart and Active Assemblies for Catalysis
Number	2013-A1
Aims	This module links molecular sciences to catalysis on complex, multicomponent and multifunctional active sites. It imparts knowledge on the interaction of active sites and active nanocatalysts with their local environment and the catalytic reaction system, and discusses cutting-edge applications in modern homogeneous and heterogeneous catalysis with the goal of understanding emerging catalytic applications for future needs.
Basics	Recommended knowledge: thematic modules T1, T2, T4 Required knowledge: Organometallic compounds, Transition metal complexes, Nanoparticles, Electronic structure (metals, oxides), Porous solids, Chirality, Catalytic chemistry and kinetics
Contents	Complex assemblies (specific synthesis, modification, structure and catalytic properties, various environments with optimised catalytic activity, selectivity and stability), Complex catalysts (functionalised mixed metal [oxide] nanoparticles, metal complexes, MOFs, immobilisation of catalysts [on solid or in liquid supports), Catalytic activation by smart assemblies (activation of unreactive molecules [CO ₂ , hydrocarbon bonds (methane), water splitting], enantioselective catalysis).
Methods	Active site assemblies (synthesis, characterisation of electronic and structural properties by molecular spectroscopy), Catalysts (spectroscopy under working conditions [ultrafast lasers], advanced testing via high-throughput experimentation), catalysis under nanconfinement and with nanostructured active components,
Type	Two-day block course/ yearly recurrence with modification
Date (month/year)	23-24 September 2013
Time	See page 2
Work load	15 hours presence/ 45 hours self-study
Examination	Written, 1 October 2013, 9:00-10:00
Credit points	2
Responsible scientists	Hey-Hawkins, Gläser, Kopinke
International guest lecturers	Ass. Prof. Jarl Ivar van der Vlugt, Prof. Dr. Andrey Karasik, Prof. Dr. Anne-Marie Caminade, Prof. Dr. Dieter Vogt, Prof. Dr. Martin Schröder, Prof. Dr. Russell Morris, Prof. Dr. Paul Wright, Prof. Dr. Vera Meynen, Prof. Dr. Petra de Jongh, Prof. Dr. Regina Palkovits, Prof. Dr. Martin Muhler, Dr. Adrian M. T. Silva, Prof. Dr. Gregory Lowry, Dr. Robert N. Grass, Prof. Dr. Harald Horn, Dr. Katrin Mackenzie, Dr. Jennifer Strunk
Industrial partners	-
Recommendations for literature, e-learning	See last pages

Minisymposium: Smart and Active Assemblies for Catalysis
23–24 September 2013

Johannes-Wislicenus-Lecture Hall (015), Faculty of Chemistry and Mineralogy,
Johannisallee 29, 04103 Leipzig

Agenda

Monday, 23 September 2013

Chair: Prof. Dr. Evamarie Hey-Hawkins

9.00–9.10 Prof. Dr. Evamarie Hey-Hawkins
(University of Leipzig, Germany)
Opening Remarks

9.10–9.55 Ass. Prof. Jarl Ivar van der Vlugt
(University of Amsterdam, The Netherlands)
Design of Reactive Ligands for Cooperative Activation of Small Molecules

9.55–10.40 Prof. Dr. Andrey Karasik
(Russian Academy of Sciences, Kazan, Russia)
Novel Phosphino Amino Pyridines for Construction of Biomimetic Catalysts for Hydrogen Economy

10.40–11.10 *Coffee Break*

Chair: Ass. Prof. Jarl Ivar van der Vlugt

11.10–11.55 Prof. Dr. Anne-Marie Caminade
(Laboratoire de Chimie de Coordination du CNRS, Toulouse, France)
Smart Nano-objects for Catalysis: Dendrimeric Catalysts

11.55–12.15 MSc Paul Neumann
(University of Leipzig, Germany)
Dendritic ferrocenyl phosphanes in redox-switchable catalysis

12.15–13.00 Prof. Dr. Dieter Vogt
(University of Edinburgh, UK)
*Building Catalysts with Molecules and Nano-objects –
From Molecules to Processes*

13.00–14.15 *Lunch Break*

Chair: Prof. Dr. Roger Gläser

14.15–15.00 Prof. Dr. Regina Palkovits (represented by Dr. Peter Hausoul)
(RWTH Aachen, Germany)
*Heterogeneous Catalysis and Renewable Feedstocks –
A Combination for the Future*

15.00–15.45 Dr. Katrin Mackenzie
(Helmholtz Centre for Environmental Research – UFZ, Germany)
Nanomaterials as Adsorbents, Reagents and Catalysts for Water Treatment

15.45–16.05 Dr. Jennifer Strunk
(Ruhr-Universität Bochum)
*Transition Metal Oxides in Mesoporous Silica: Structural Characterization,
Adsorption and Photocatalysis*

16.05–16.35 *Coffee Break*

Chair: Prof. Dr. Paul Wright

16.35–17.20 Prof. Dr. Martin Schröder
(University of Nottingham, UK)
Porous Metal-Organic Materials for Gas Storage and Selectivity

17.20–18.05 Prof. Dr. Russell Morris
(University of St Andrews, UK)
Manipulating Zeolites and MOFs for Application

18.10–20.00 *Poster Session (with Drinks and Fingerfood)*

Tuesday, 24 September 2013

Chair: Prof. Dr. Martin Schröder

9.00–9.45 Prof. Dr. Paul Wright
(University of St Andrews, UK)
*Designed Synthesis, Adsorption and Catalytic Performance of Structurally
Flexible MOFs and Zeolites*

9.45–10.30 Prof. Dr. Harald Horn
(Karlsruhe Institute of Technology, Germany)
*Sorption of magnetic nanoparticles on biofilm structures and identification
with MRI*

10.30–11.00 *Coffee Break*

Chair: Prof. Dr. Gregory Lowry

- 11.00–11.45 Prof. Dr. Petra de Jongh
(Utrecht University, The Netherlands)
The Impact of Collective Properties on the Stability of Supported Nanoparticles for Catalytic and Sustainable Energy Applications
- 11.45–12.05 Dr. Alina M. Balu
(Aalto University, Finland)
Novel mechanochemical synthesis of magnetic functionalized mesoporous SBA-15 nanocomposites
- 12.05–12.50 Prof. Dr. Vera Meynen
(University of Antwerp, Belgium)
Controlled synthesis of multimodal materials, creating designed materials properties for catalysis

12.50–14.00 *Lunch Break*

Chair: Prof. Dr. Vera Meynen

- 14.00–14.20 Jasper Lefevere
(Flemish Institute for Technological Research (VITO N.V.) and University Antwerp, Belgium)
Synthesis of hierarchically porous ZSM-5 catalyst for methanol-to-olefins
- 14.20–15.05 Prof. Dr. Martin Muhler
(Ruhr-Universität Bochum, Germany)
Carbon Nanotubes – Synthesis, Functionalization, and Applications in Heterogeneous Catalysis
- 15.05–15.50 Dr. Adrian M. T. Silva
(University of Porto, Portugal)
Carbon-based Materials as Catalysts for Water Treatment

15.50–16.20 *Coffee Break*

Chair: Prof. Dr. Frank-Dieter Kopinke

- 16.20–17.05 Prof. Dr. Gregory Lowry
(Carnegie Mellon University, Pittsburgh, Pennsylvania, USA)
Optimizing Fe⁰-based in situ groundwater remediation agents
- 17.05–17.50 Dr. Robert N. Grass
(ETH Zurich, Switzerland)
Smart (Nano)materials Interfacing Biochemistry: Moving Molecules and Tracing Polymers



17.50–18.10 Prof. Dr. Evamarie Hey-Hawkins
Award Ceremony
Closing Remarks

18.10–20.00 *Get Together*

Recommendations for literature:

Jarl Ivar van der Vlugt

J.I. van der Vlugt, Eur. J. Inorg. Chem. 2012, 363-375; J.I. van der Vlugt, J.N.H. Reek, Angew. Chem. Int. Ed. 2009, 48, 8832-8846
 R. Lindner, B. van den Bosch, M. Lutz, J.N.H. Reek, J.I. van der Vlugt, Organometallics 2011, 30, 499-510; S.Y. de Boer, Y. Gloaguen, J.N.H. Reek, M. Lutz, J.I. van der Vlugt, Dalton Trans. 2012, 41, 11276-11283

Anne-Marie Caminade

Pyrene-Tagged Dendritic Catalysts Noncovalently Grafted onto Magnetic Co/C Nanoparticles: An Efficient and Recyclable System for Drug Synthesis. M. Keller, V. Collière, O. Reiser, A.-M. Caminade, J.-P. Majoral, A. Ouali Angewandte Chemie, International Edition, 2013, 52 (13): 3626-3629

An efficient and recyclable dendritic catalyst able to dramatically decrease palladium leaching in Suzuki couplings. M. Keller, A. Hameau, G. Spataro, S. Ladeira, A.-M. Caminade, J.-P. Majoral, A. Ouali Green Chemistry, 2012, 14 (10): 2807-2815

Dieter Vogt

M. Janssen, C. Müller, D. Vogt, Recent advances in recycling of homogeneous catalysts using membrane separation, Green Chem. 2011, 13, 2247-2257;
 M. Janssen, J. Wilting, C. Müller, D. Vogt, Continuous Rh-catalyzed hydroformylation of 1-octene with POSS-enlarged PPh₃, Angew. Chem. Int. Ed. 2010, 49, 7738-7741;
 M. Janssen, C. Müller, D. Vogt, Dalton Trans. 2010, 36, 8403-8411
 (Molecular weight enlargement—a molecular approach to continuous homogeneous catalysis)

Vera Meynen

Jarian Vernimmen, Vera Meynen and Pegie Cool: Synthesis and catalytic applications of combined zeolitic/mesoporous materials, *Beilstein J. Nanotechnol.* 2011, 2, 785–801;
 Jarian Vernimmen et al.: Immersion Calorimetry as a Tool To Evaluate the Catalytic Performance of Titanosilicate Materials in the Epoxidation of Cyclohexene, [dx.doi.org/10.1021/la104808v](https://doi.org/10.1021/la104808v)

Petra de Jongh

Nanosizing and confinement: new strategies towards meeting hydrogen storage goals, P. E. de Jongh, P. Adelhelm, ChemSusChem 3 (2010) 1332-1348.
 Towards stable catalysts by control over the collective features of supported metal nanoparticles, G. Prieto, J. Zecevic, H. Friedrich, K.P. de Jong, P.E. de Jongh, Nature Mater. 12 (2013), 34-39.

Martin Muhler

Michael J. Becker et al.: Separating the initial growth rate from the rate of deactivation in the growth kinetics of multi-walled carbon nanotubes from ethene over a cobalt-based bulk catalyst in a fixed-bed reactor, C A R B O N 5 8 (2 0 1 3) 1 0 7 – 1 1 5,
[http://dx.doi.org/10.1016/j.carbon.2013.02.038](https://doi.org/10.1016/j.carbon.2013.02.038)

Shankhamala Kundu, Yuemin Wang, Wei Xia, and Martin Muhler: Thermal Stability and Reducibility of Oxygen-Containing Functional Groups on Multiwalled Carbon Nanotube Surfaces: A Quantitative High-Resolution XPS and TPD/TPR Study, *J. Phys. Chem. C*, 2008, 112 (43), 16869-16878, DOI: 10.1021/jp804413a

Adrian M.T. Silva

Pastrana-Martínez, L.M., Morales-Torres, S., Likodimos, V., Figueiredo, J.L., Faria, J.L., Falaras, P., Silva, A.M.T. (2012). Advanced nanostructured photocatalysts based on reduced graphene oxide-TiO₂ composites for degradation of diphenhydramine pharmaceutical and methyl orange dye, *Applied Catalysis B: Environmental*, 123-124, 241-256, doi: 10.1016/j.apcatb.2012.04.045.

Marques, R.R.N., Machado, B.F., Faria, J.L., Silva, A.M.T. (2010). Controlled generation of oxygen functionalities on the surface of Single-Walled Carbon Nanotubes by HNO₃-hydrothermal oxidation, *Carbon*, 48(5), 1515-1523. doi: 10.1016/j.carbon.2009.12.047.

Greg Lowry

Teresa L. Kirschling et al.: Impact of Nanoscale Zero Valent Iron on Geochemistry and Microbial Populations in Trichloroethylene Contaminated Aquifer Materials, *Environ. Sci. Technol.* 2010, 44, 3474–3480;

Tanapon Phenrat, Yueqiang Liu, Robert D. Tilton, and Gregory V. Lowry: Adsorbed Polyelectrolyte Coatings Decrease Fe₀ Nanoparticle Reactivity with TCE in Water: Conceptual Model and Mechanisms, *Environ. Sci. Technol.*, 2009, 43 (5), 1507-1514, DOI: 10.1021/es802187d;

Tanapon Phenrat et al.: Polymer-Modified Fe₀ Nanoparticles Target Entrapped NAPL in Two Dimensional Porous Media: Effect of Particle Concentration, NAPL Saturation, and Injection Strategy, dx.doi.org/10.1021/es200577n, *Environ. Sci. Technol.* 2011, 45, 6102–6109;

Navid Saleh et al.: Adsorbed Triblock Copolymers Deliver Reactive Iron Nanoparticles to the Oil/Water Interface, *NANO LETTERS* 2005, Vol. 5, No. 12, 10.1021/nl0518268 CCC

Robert Grass

Robert N. Grass, Evagelos K. Athanassiou, and Wendelin J. Stark: Covalently Functionalized Cobalt Nanoparticles as a Platform for Magnetic Separations in Organic Synthesis, *Angew. Chem. Int. Ed.* 2007, 46, 4909 –4912;

Daniela Paunescu, Roland Fuhrer, and Robert N. Grass: Protection and Deprotection of DNA—High-Temperature Stability of Nucleic Acid Barcodes for Polymer Labeling, *Angew. Chem. Int. Ed.* 2013, 52, 4269 –4272;

Harald Horn

Bertram Manz, Frank Volke, Daniel Goll, Harald Horn: Measuring Local Flow Velocities and Biofilm

Structure in Biofilm Systems With Magnetic Resonance Imaging (MRI), DOI: 10.1002/10782;

Michael Wagner, Bertram Manz, Frank Volke, Thomas R. Neu, Harald Horn: Online Assessment of Biofilm Development, Sloughing and Forced Detachment in Tube Reactor by Means of Magnetic Resonance Microscopy, *Biotechnology and Bioengineering*, Vol. 107, No. 1, September 1, 2010, DOI 10.1002/bit.22784