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Unifying Concepts in Catalysis

BIG NSE

BIG-NSE Minisymposium

16th-17th June 2010, TU Berlin

Biological and (electro-) chemical catalysts for hydrogen conversion

For the workshop, please sign up via mail to: lars.lauterbach@biologie.hu-berlin.de

Wednesday 16th June			
13:30	**Workshop**		
13:30- 13:45	Opening words	Lars Lauterbach / Oliver Lenz	Room TC 033
13:45-14:15	Iron transport and delivery for hydrogenase in Escherichia coli	**Constanze Pinske** (Group of Gary Sawers, Martin-Luther University Halle-Wittenberg)	
14:15- 14:45	Assembly of the active site in hydrogenases	**Ingmar Bürstel** (Bärbel Friedrich/ Oliver Lenz, HU Berlin)	
14:45- 15:15	*Coffee & Tea*		
15:15	Chair: Marc Fontecave		
15:15 -15:45	Electrochemical Water Splitting- From Theory to Materials	**Tobias Reier** (Peter Strasser, TU Berlin)	
15:45-16:15	Structural changes of a H_2-evolving nickel catalyst due to grafting on a carbon electrode	**Jonathan Heidkamp** (Holger Dau, FU Berlin)	
16:15- 16:45	Oxygen reduction on well-defined core-shell $PtCu_3$ and $PtCo_3$ electrocatalyst.	**Mehtap Özaslan** (Peter Strasser, TU Berlin)	
16:45- 17:15	*Break*		
17:15- 18:45	**UniCat Lecture**: From enzymes to nanocatalysts: the case of hydrogenases	**Prof. Dr. Marc Fontecave** (Laboratoire Chimie et Biologie des Métaux, CEA Grenoble, France)	**Room C 243**

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Thursday 17th June			
10:00	**Workshop**		
10:00	Chair: Marc Fontecave		
10:00-10:30	Beta-Diketiminato Nickel Complexes and H_2 Activation	**Stefan Pfirrmann** (Christian Limberg, HU Berlin)	**Room TC 033**
10:30-10:45	*Coffee& Tea*		
10:45-11:15	Study of non-noble metal electrocatalyst for PEM fuel cell	Frédéric Hasché (Peter Strasser, TU Berlin)	
11:15-11:45	The oxygen evolution reaction of a cobalt film catalyst probed by synchrotron X-ray radiation	**Marcel Risch** (Holger Dau, FU Berlin)	
11:45-13:00	*Lunch*		
13:00	Chair: Kylie Vincent		
13:00-13:30	The *Ralstonia eutropha* membrane-bound [NiFe]-hydrogenase - an overview	**Dr. Stefan Frielingsdorf** (Bärbel Friedrich, HU Berlin)	
13:30-14:00	A combined *in situ* and *in vitro* EPR and FTIR spectroscopic study on the soluble, NAD^+-reducing hydrogenase from *Ralstonia eutropha* H16	**Marius Horch** (Peter Hildebrandt/ Ingo Zebger, TU Berlin)	
14:00-14:15	*Coffee& Tea*		
14:15-14:45	Impact of cofactor composition and interactions on hydrogenase-catalysed NAD^+ reduction	**Lars Lauterbach** (Bärbel Friedrich/ Oliver Lenz, HU Berlin)	
14:45-15:15	Activity and stability of the hydrogen oxidising and NAD^+ reducing soluble hydrogenase from *Ralstonia eutropha* H 16 with special regard to technical use	**Juliane Ratzka** (Marion Ansorge-Schumacher, TU Berlin)	
15:15-16:15	*Break*		
16:15-17:45	**UniCat Lecture**: Studying and exploiting [NiFe]-hydrogenases under electrochemical control	**Dr. Kylie Vincent** (University of Oxford, UK)	**Room C 243**

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UniCat Lecture

(Actual changes on: www.unicat.tu-berlin.de/Event)

Lecturer: **Prof. Dr. Marc Fontecave**, Laboratoire de Chimie et Biologie des Métaux, CEA Grenoble, France

Title: **From enzymes to nanocatalysts: the case of hydrogenases**

Abstract: One of the grand challenges of twenty-first century chemistry is to convert abundant energy-poor molecules to energy rich molecules using sunlight as the energy source. Hydrogen from water is such a solar fuel. However its production and use currently depend on noble metals such as Platinum which is expensive and not abundant enough. Viable renewable energy systems will require new catalysts made from earth-abundant materials, cheap and robust. We will describe our bioinspired strategy, aiming at reproducing hydrogenase active sites, which leads to remarkable Cobalt-based and Nickel-based (photo) catalysts for hydrogen production.

Date: **Wednesday, 16 June 2010**

Time: **5:15 pm - around 6:45 pm**

Location: **TU Berlin**
Institute of Chemistry,
Building C
Straße des 17. Juni 115,
10623 Berlin
room C 243

Organiser: Dr. Oliver Lenz (HUB)
Lars Lauterbach (BIG-NSE Student)

Coffee and tea will be served thirty minutes prior to the lecture start.
Guests are cordially invited to attend!

Prof. Dr. Matthias Driess, Chair of the Cluster of Excellence UniCat

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UniCat Lecture

(Actual changes on: www.unicat.tu-berlin.de/Event)

Lecturer: **Dr. Kylie Vincent**, Inorganic Chemistry Laboratory, University of Oxford, UK

Title: **Studying and exploiting [NiFe]-hydrogenases under electrochemical control**

Abstract: Microbial hydrogenase enzymes are highly active catalysts for H_2 oxidation or H_2 production, employing iron or nickel-iron active sites coordinated by CO, CN^- and thiolate ligands. An electron relay chain of iron-sulfur clusters provides efficient transport of electrons between the buried active site and the protein surface. Direct electrochemical experiments in which a hydrogenase is adsorbed onto a pyrolytic graphite electrode provide precise control over catalytic activity and interconversions between active and inactive states of the enzymes. These reactions depend critically on potential, and set the potential window in which a given hydrogenase is active. Electrochemical experiments also provide information on catalytic bias (H^+ reduction vs H_2 oxidation), O_2 tolerance, catalytic selectivity for H_2 over other small molecules, inhibition, and affinity for H_2. Insight into the chemistry of NiFe hydrogenases from a range of organisms will be discussed.

Spectroscopic experiments on hydrogenases have mostly been carried out in solution, relying on slow diffusion of electron transfer mediators. Infrared (IR) spectroscopy has been widely utilised because the CO and CN ligands at hydrogenase active sites give rise to fairly intense vibrational bands in the IR spectrum, and the position of these bands is sensitive to electronic and coordination changes at the metals. There is now a need for methods that couple IR sampling with direct electrochemical control. Metal electrodes are convenient for IR spectroscopic study of surface species, and methods have been reported for spectroelectrochemical study of proteins on gold. Graphite has been the most successful electrode material for direct electrochemical experiments on hydrogenases, however, and we are working to develop a surface spectroscopic approach for analysing hydrogenase chemistry controlled at a graphite electrode.

Together, direct electrochemical and spectroelectrochemical methods are contributing to a picture of the catalytic characteristics required for exploitation of hydrogenases or bio-inspired catalysts[4] in energy technologies.

Date: **Thursday, 17 June 2010**

Time: **4:15 pm - around 5:45 pm**

Location: **TU Berlin, Institute of Chemistry, Building C, Straße des 17. Juni 115, 10623 Berlin, room C 243**

Organiser: Dr. Oliver Lenz (HUB)
Lars Lauterbach (BIG-NSE Student)

Coffee and tea will be served thirty minutes prior to the lecture start.
Guests are cordially invited to attend!

Prof. Dr. Matthias Driess, Chair of the Cluster of Excellence UniCat