BASF – The Chemical Company
We create chemistry for a sustainable future

- Sales 2012: 72 129 million €
- EBIT 2012: 6 647 million €
- worldwide 110 782 employees
- 6 verbund sites and approx. 380 production sites worldwide
BASF – The Chemical Company
Organization

Segments and Divisions as of January 1, 2013

- Chemicals
  - Petrochemicals
  - Monomers
  - Intermediates

- Performance Products
  - Dispersions & Pigments
  - Care Chemicals
  - Nutrition & Health

- Functional Materials & Solutions
  - Catalysts
  - Construction Chemicals
  - Nutrition & Health

- Agricultural Solutions
  - Crop Protection
  - Coatings
  - Performance Materials

- Oil & Gas
  - Oil & Gas

August 2013
TriesteDFT & beyond Workshop / michael.rieger@basf.com
Innovation at BASF
R&D 2012 at a Glance

Research for the future: with our innovative products and processes, we provide sustainable solutions for global challenges.

- Expenditures for R&D circa €1.73 billion, world leader in chemical industry
- Since 2005 increase of R&D expenditures up to 60%
- Around 3,000 projects, 10500 employees
- Strongest innovation power in the chemical industry (No.1 in the Patent Asset Index™)
- Sales target 2020: circa €30 billion from product innovations

<table>
<thead>
<tr>
<th>Category</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Chemicals</td>
<td>10 %</td>
</tr>
<tr>
<td>2 Performance Products</td>
<td>20 %</td>
</tr>
<tr>
<td>3 Functional Materials &amp; Solutions</td>
<td>20 %</td>
</tr>
<tr>
<td>4 Agricultural Solutions</td>
<td>25 %</td>
</tr>
<tr>
<td>5 Oil &amp; Gas</td>
<td>2 %</td>
</tr>
<tr>
<td>6 Corporate Research, others</td>
<td>23 %</td>
</tr>
</tbody>
</table>
We Create Chemistry
From Chemicals to Chemistry

Tasks

- Chemistry as key enabler for functionalized materials & solutions
- Interdisciplinary approach
- Deep understanding of customer value chains required

From chemicals to chemistry: the innovation focus changed
The Future of the Chemical Industry
Demographic Challenges Set the Stage

Nine billion people in 2050 but only one earth

Resources, Environment & Climate
Food & Nutrition
Quality of life

Chemistry as enabler
The Future of the Chemical Industry
Many Growth Opportunities

Nine billion people in 2050 but only one Earth

Chemistry as enabler

Sustainability and innovation as main driver
Innovation focus on materials & solutions
Growth of chemical production above GDP
60% of chemical production in emerging countries
# Chemistry-Based Innovations

**Growth and Technology Fields**

<table>
<thead>
<tr>
<th>Resources, Environment &amp; Climate</th>
<th>Food &amp; Nutrition</th>
<th>Quality of life</th>
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</table>

## Chemistry as enabler

<table>
<thead>
<tr>
<th>Key Customer Sectors</th>
<th>Transportation</th>
<th>Construction</th>
<th>Consumer Goods</th>
<th>Health &amp; Nutrition</th>
<th>Electronics</th>
<th>Agriculture</th>
<th>Energy &amp; Resources</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Growth Fields*</th>
<th>Batteries for Mobility</th>
<th>Heat Management</th>
<th>Enzymes</th>
<th>Medical Solutions</th>
<th>Organic Electronics</th>
<th>Plant Biotechnology</th>
<th>E-Power Management</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lightweight Composites</td>
<td></td>
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</tr>
</tbody>
</table>

## Technology Fields

<table>
<thead>
<tr>
<th>Materials, Systems &amp; Nanotechnology</th>
<th>Raw Material Change</th>
<th>White Biotechnology</th>
</tr>
</thead>
</table>

*including growth fields still under evaluation
Innovation
Global Know-How Verbund

Thanks to our close cooperation with numerous partners from science and business worldwide, we have created an international and interdisciplinary Know-How Verbund.

- Approx. 10,500 employees in R&D worldwide
- Know-How Verbund with about 600 excellent universities, research institutions and companies
Global Know-How Verbund
Inside BASF and with Partners

BASF R&D Sites
R&D Cooperations

Cambridge
Karlsruhe
Düsseldorf
Strasbourg
Mumbai
Heidelberg
Basel
Ludwigshafen
Singapore
Shanghai
Wyandotte
Raleigh
Iselin
Guaratinguetá

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Technology Platform
Advanced Materials & Systems Research

We develop functional materials and system solutions for a sustainable future targeting the automotive, construction, home & personal care, packaging, water and wind industry.

Competencies

- Develop new structural and functional materials, additives, dispersions as well as composites and hybrid systems
- Optimize products and processes, develop new smart-scale production concepts
- Provide comprehensive characterization and modeling methods and establish structure-property relationships

Innovation examples

- Advanced composite materials for new lightweight concepts of load-bearing car parts and high-performance wind rotor blades
- System solutions for water purification based on flocculants, anti-fouling additives and polymeric membrane materials
Technology Platform
Biological & Effect Systems Research

We develop new active substances, methods, processes and systems for a wide range of applications, e.g. in crop protection, pharma, nutrition and energy management.

Competencies
- New chemical and biological crop protection products
- Efficient and energy-conserving production of (bio)chemicals
- Materials and systems for lighting, displays & energy conversion
- Modeling and formulation
- Development of alternative methods in toxicology

Innovation examples
- Development of crop protection blockbusters, e.g. F 500®, Kixor®, Xemium®
- Biotechnological production of vitamin B$_2$ and enzymes for animal nutrition, biopolymer Schizophyllan for enhanced oil recovery
- Organic solar cells for the concept-car smart forvision
We develop new technologies and processes and optimize existing processes for the manufacture of basic chemicals, intermediates and fine chemicals.

Competencies
- Synthesizing basic chemicals, intermediates, fine chemicals and new materials
- Chemical, refinery and environmental catalysis
- Battery components and electrochemistry
- Process development and unit operations

Innovation examples
- Resource-efficient process for the synthesis of propylene oxide (HPPO)
- Improved lithium-ion batteries and new battery concepts
Computational Competence Centers in R&D Organization

- Quantum Chemistry
- Fluid Mechanics
- Reaction Technology
- Scientific Computing
- BASF Research Verbund
- Polymer Reaction Engin.
- Computational Chemistry and Biology
- Bioinformatics
- Polymer Modeling

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Battery materials of BASF will enhance battery life-time and reduce cost with no compromises on safety.

Existing activities

- Chemicals and materials for lithium-ion batteries (cathode and anode materials, electrolytes, binders, solvents)
- Work on concepts for next generations of batteries (lithium-sulfur, lithium-air)
- Establishing the global business unit “Battery Materials”

Targets

- Position BASF as a leading materials and components supplier by utilization of technology and business synergies
- Find innovative solutions for future mobility
Applications of Modeling to Growth Fields
Organic Electronics

**BASF provides material systems solutions for mass applications in organic electronics.**

**Existing activities**
- Material systems for OLEDs (displays and lighting)
- Printable materials for circuit boards and displays
- Contract manufacturing of organic dopants for display applications

**Targets**
- Position BASF as provider of material solutions for next generation displays and lighting
- Creating system know-how and technology synergies in synthesis, formulation and up-scaling
- Enter new markets based on BASF’s core competencies
Applications of Modeling to Technology Fields
Raw Material Change (Catalysis)

We work on sustainable processes for using alternative raw materials such as natural gas, biomass and CO₂.

Research focus

- Increased use of natural gas, biomass and CO₂ as basis for raw materials
- Integration of competencies: synthesis, catalysis, process development and unit operations, high-throughput methods

Examples of existing activities

- Natural gas:
  Olefins from natural gas by using dehydrogenation technologies
- Carbon dioxide (CO₂):
  Synthesis of formic acid and acrylates
- Biomass:
  Lignocellulose as a raw material
Homogeneous Catalysis -
Quantum Chemical Catalyst Screening
(work by A. Schäfer)

Hydroformylation of Olefins

Reaction:
\[ R \text{C} + \text{CO} + \text{H}_2 \xrightarrow{\text{Co, Rh cat.}} R\text{CHO} \]

Olefin

Catalyst:

Goal:
Design catalysts for n-selectivity

5-600 bar
iso-Aldehyde
n-Aldehyde

desired product

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The catalyst in action - a molecular production machine

Catalyst

Olefin insertion

simulated catalytic cycle
Reaction pathway and selectivity

\[ S \sim \exp \left( \frac{\Delta\Delta G^\ddagger}{RT} \right) \]

desired product

n-product

i-product

[\text{G} / \text{kJ mol}]

\begin{itemize}
  \item + Olefin
  \item - CO
  \item + CO
  \item + H$_2$
  \item - Aldehyde
\end{itemize}
Screening for optimal ligands using the identified descriptor

Comparison of calculated and experimental selectivities [%]

<table>
<thead>
<tr>
<th></th>
<th>Experiment</th>
<th>Calculation</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\text{PPh}_2)</td>
<td>66.5</td>
<td>75.0</td>
</tr>
<tr>
<td>(\text{Ph}_2\text{P})</td>
<td>89.6</td>
<td>97.8</td>
</tr>
<tr>
<td>(\text{PPh}_2)</td>
<td>99.0</td>
<td>99.3</td>
</tr>
</tbody>
</table>

In collaboration with Prof. Hofmann, Uni Heidelberg

BASF Patent
Application: Lifetime prediction using short-time experiments
The catalyst particles change shape in the process.

**fresh catalyst**

**aged catalyst**

(14 months)

*optimal Ag particle size*  
~ 100nm

Caused by a complicated set of microscopic processes

- Particle translation
- Particle rolling
- Particle flow
- Atom/cluster migration on surface
- Atom/cluster migration in gas phase
- Particle coalescence
First step – the particle shape
(work done together with Monica Garcia-Mota)

• Prediction of the equilibrium composition and shape of supported Ag nanoparticles on $\alpha$-Al$_2$O$_3$

Ag-Al$_2$O$_3$ interaction
Predictions using a theoretical approach

First-principles thermodynamic study

Surface free energy

\( \gamma(T, p) \)

Multi-component system being in equilibrium with atomic reservoirs

stable surface at

\((p, T)\)

bridging the pressure and temperature gap

THEORY

EXPERIMENTS
Equilibrium Ag surface

First-principles thermodynamic study

- Ag(111)
- 1/16ML
- 1/9ML
- 3/16ML
- 2/9ML
- 1/4ML
- \(\text{Ag}_2\text{O}/\text{Ag(111)}^*\)
- \(\text{Ag}_2\text{O}(111)\)

Graph showing the dependence of surface energy (\(\gamma\)) on the chemical potential difference (\(\Delta\mu_O\)) for different Ag surfaces under oxygen pressure at 1 atm and 500K.

\(\gamma_{111}\)
Equilibrium $\alpha$-$\text{Al}_2\text{O}_3$ (0001) surface
Equilibrium $\alpha$-Al$_2$O$_3$ (0001) surface
Equilibrium $\alpha$-Al$_2$O$_3$ (0001) surface with Ag coverage

$\Delta \mu_{H_2O}(eV)$

$\gamma$(meV/$\text{Å}^2$)

$H_2O$ pressure at $T=500$K (atm)

$p_{O_2}=1$ atm

$p_{H2O} < 10^{-5}$ atm

$\text{pH}_2O< 10^{-5}$ atm
Shape of supported Ag nanoparticles on α-Al₂O₃
Wulff-Kaishew construction

- Ag surface free energies

\[ H = c(\gamma_{111} + \gamma^*) \]

\[ \gamma^* = \gamma_{metal} + \frac{E_{adh}}{A} \]

- Effective surface energy

- Equilibrium Al₂O₃ surface
Bringing it all together: Example particle shapes

$\text{AlO}_3\text{Al-R}$
- $c_{\gamma^*} > 0$
- $c_{\gamma^*} < c_{\gamma_{111}}$

$\text{H}_3\text{O}_3\text{Al-R}$
- $c_{\gamma^*} > 0$
- $c_{\gamma^*} > c_{\gamma_{111}}$

$T=500K$
$p_{O_2}=1\text{atm}$

$p_{H_2O} < 10^{-6} \text{ atm}$

$\sim 77 \%$

$p_{H_2O} > 10^{-6} \text{ atm}$

$\sim 70 \%$

$\sim 23 \%$

$\sim 30 \%$
Next steps

Study the influence of **promoters**

% Ag (100) \rightarrow selectivity

binding energies \rightarrow sintering

Macroscopic modeling of particle size distributions

Using a sinterkernel, e.g.

\[ \beta(x, y) = \beta_0 \cdot (x^{-m} + y^{-m}) \]
OLEDs - Multiscale Modeling of Devices
(work by C. Lennartz)

picture taken from J. Mat. Chem. 12, 10971
cooperation BASF (Lennartz) & MPIP (Adrienko)
High Temperature PEM fuel cell degradation
(work by A. Badinski)

hydrogen oxidation reaction
\[ \text{H}_2 \rightarrow 2\text{H}^+ + 2\text{e} \]

oxygen reduction reaction
\[ 0.5 \text{O}_2 + 2\text{e} \rightarrow \text{O}^- \]

Main degradation mechanisms
- Ostwald ripening
  ⇒ effects activity of catalyst
- reduction of \( \text{H}_3\text{PO}_4 \) acid
  ⇒ effects proton transport

platinum particle catalyst
The fuel cell model

Model consists of

2 measurement functions

12 model parameters

2 ordinary differential equations

4 experimental controls:

T, inlet-flow (H₂,O₂,N₂)
Goodness-of-fit
Parameter covariance analysis

Model/data deviation explained by statistical errors with p=99.96% average parameter uncertainties less then 5%
Model predictions
choose Ohmic resistivity as an example

Model/data deviation explained by statistical errors with $p=1e-6\%$ (Set 1)
Model recalibrated with Ohmic resistivity data (Set 2)
Thank you for your attention.

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