

An Introduction to Catalysis and Surface Science

Science dialogue with the students of Tsuru high school in
Yamanashi prefecture.

Dr. Mathias Laurin

Research Centre for Spectrochemistry
Graduate School of Science
The University of Tokyo
Hongo, 7-3-1 Bunkyo-ku,
Tokyo 113-0033, Japan

12 June 2007

Table of Contents

Introduction

Catalysis

What is catalysis?

Homogeneous or heterogeneous catalysis

Example of heterogeneous catalysis

Ingeneering?

Surface Science

Complex surfaces

Complex reactions at complex surfaces

Intelligent materials

Windows

Nanotechnologies

Outline

Introduction

Catalysis

What is catalysis?

Homogeneous or heterogeneous catalysis

Example of heterogeneous catalysis

Ingeneering?

Surface Science

Complex surfaces

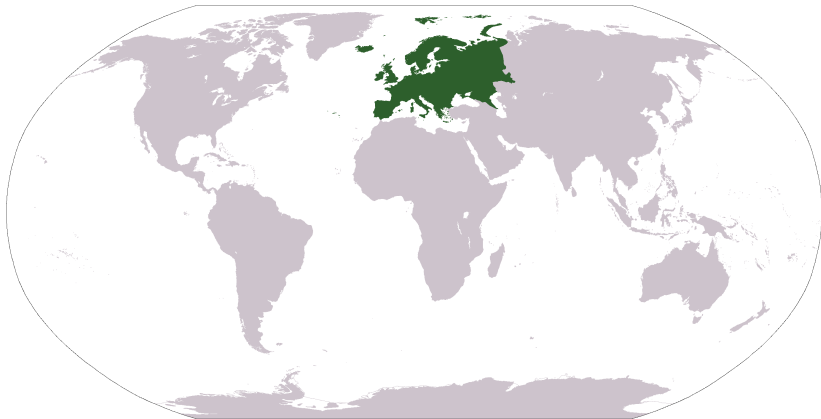
Complex reactions at complex surfaces

Intelligent materials

Windows

Nanotechnologies

Location of Europe



Satellite view of Europe



Dijon, where I was born. . .



Dijon, where I was born...



... and where I studied

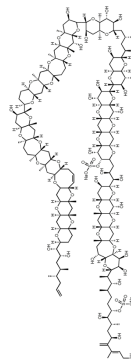
Université de Bourgogne

DEUG Biologie organic chemistry

Licence de Chimie inorganic chemistry

Maîtrise Matériau materials science

DEA Chimie-physique materials science and
physical chemistry



... and where I studied

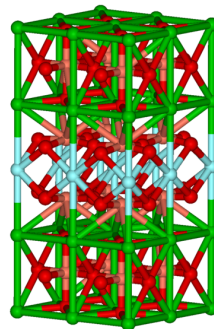
Université de Bourgogne

DEUG Biologie organic chemistry

Licence de Chimie inorganic chemistry

Maîtrise Matériau materials science

DEA Chimie-physique materials science and
physical chemistry



... and where I studied

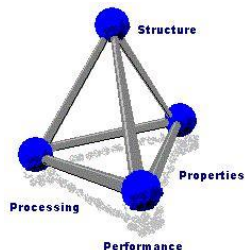
Université de Bourgogne

DEUG Biologie organic chemistry

Licence de Chimie inorganic chemistry

Maîtrise Matériau materials science

DEA Chimie-physique materials science and
physical chemistry



... and where I studied

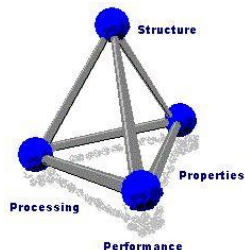
Université de Bourgogne

DEUG Biologie organic chemistry

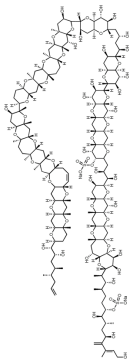
Licence de Chimie inorganic chemistry

Maîtrise Matériau materials science

DEA Chimie-physique materials science and
physical chemistry

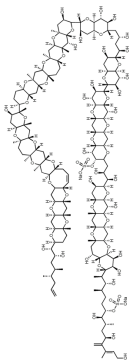


From chemistry to materials science

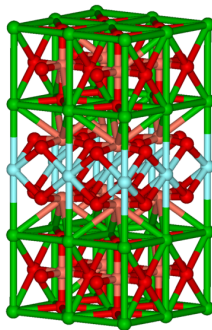


Pharmacy, food,
petrochemicals. . .

From chemistry to materials science

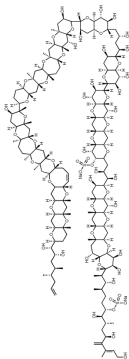


Pharmacy, food,
petrochemicals. . .

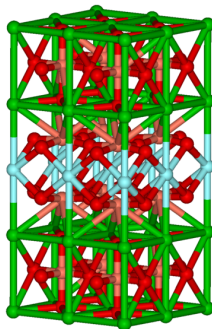


Environment,
minerals, solid
state. . .

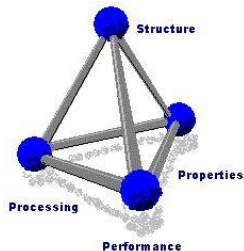
From chemistry to materials science



Pharmacy, food,
petrochemicals. . .



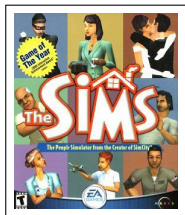
Environment,
minerals, solid
state. . .



Plastics, metallurgy,
ceramics, polymers. . .

Chemometrics at the Katholieke Universiteit Nijmegen

Applying artificial intelligence. . .



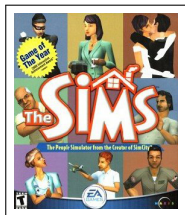
The Sim's



Kasparov vs.
Deep Blue

Chemometrics at the Katholieke Universiteit Nijmegen

Applying artificial intelligence. . .



The Sim's



Kasparov vs.
Deep Blue



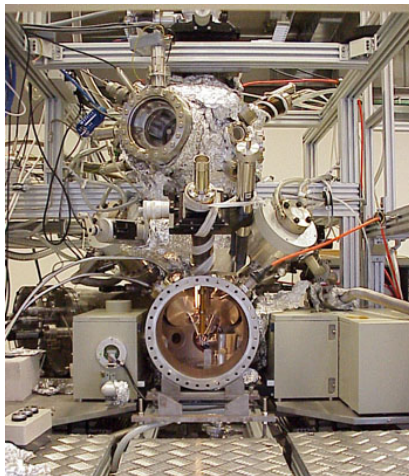
MRI Brain tumor

. . . to biology and chemistry.

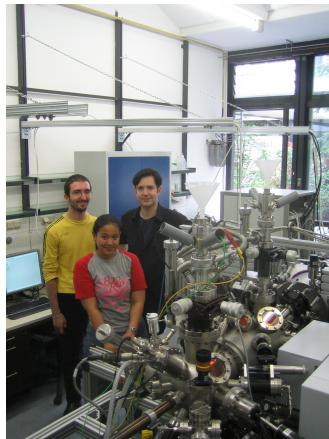
Berlin



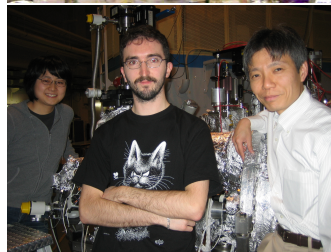
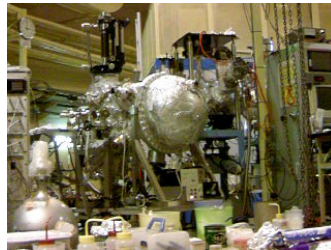
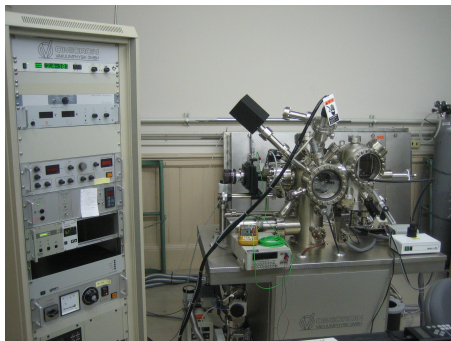
Fritz-Haber-Institut der Max-Planck-Gesellschaft



Erlangen: Building a UHV apparatus



The University of Tokyo



Outline

Introduction

Catalysis

What is catalysis?

Homogeneous or heterogeneous catalysis

Example of heterogeneous catalysis

Ingeneering?

Surface Science

Complex surfaces

Complex reactions at complex surfaces

Intelligent materials

Windows

Nanotechnologies

What is catalysis?

All chemical processes in biology and chemistry rely on catalysis.

In a (bio)chemical process, catalysis

- ▶ modifies the kinetics for the reaction;
- ▶ modifies the pathway of the reaction;
- ▶ tunes a reaction toward a specific product.

The catalyst will modify the way the reaction is performed but will be involved in neither reactants nor products.

What is catalysis?

All chemical processes in biology and chemistry rely on catalysis.

In a (bio)chemical process, **catalysis**

- ▶ modifies the kinetics for the reaction;
- ▶ modifies the pathway of the reaction;
- ▶ tunes a reaction toward a specific product.

The catalyst will modify the way the reaction is performed but will be involved in neither reactants nor products.

What is catalysis?

All chemical processes in biology and chemistry rely on catalysis.

In a (bio)chemical process, **catalysis**

- ▶ modifies the **kinetics** for the reaction;
- ▶ modifies the pathway of the reaction;
- ▶ tunes a reaction toward a specific product.

The catalyst will modify the way the reaction is performed but will be involved in neither reactants nor products.

What is catalysis?

All chemical processes in biology and chemistry rely on catalysis.

In a (bio)chemical process, **catalysis**

- ▶ modifies the kinetics for the reaction;
- ▶ modifies the **pathway** of the reaction;
- ▶ tunes a reaction toward a specific product.

The catalyst will modify the way the reaction is performed but will be involved in neither reactants nor products.

What is catalysis?

All chemical processes in biology and chemistry rely on catalysis.

In a (bio)chemical process, **catalysis**

- ▶ modifies the kinetics for the reaction;
- ▶ modifies the pathway of the reaction;
- ▶ **tunes** a reaction toward a specific product.

The catalyst will modify the way the reaction is performed but will be involved in neither reactants nor products.

What is catalysis?

All chemical processes in biology and chemistry rely on catalysis.

In a (bio)chemical process, catalysis

- ▶ modifies the kinetics for the reaction;
- ▶ modifies the pathway of the reaction;
- ▶ tunes a reaction toward a specific product.

The catalyst will modify the **way** the reaction is performed but will be involved in **neither reactants nor products**.

History (wikipedia)

*The phrase catalysis was coined by Jöns Jakob Berzelius who in 1835 was the first to note that **certain chemicals speed up** a reaction. Other early chemists involved in catalysis were Alexander Mitscherlich who in 1831 referred to contact processes and Johann Wolfgang Döbereiner who spoke of contact action and whose lighter based on hydrogen and a platinum sponge became a huge commercial success in the 1820s. In the 1880s, Wilhelm Ostwald at Leipzig University started a series of systematic investigations into reactions that were catalyzed by the presence of acids and bases, and found both that chemical reactions occur at finite rates, and that these rates can be used to determine the strengths of acids and bases. For this work, Ostwald was awarded the 1909 Nobel Prize in Chemistry.*

History (wikipedia)

*The phrase catalysis was coined by Jöns Jakob Berzelius who in 1835 was the first to note that certain chemicals speed up a reaction. Other early chemists involved in catalysis were Alexander Mitscherlich who in 1831 referred to **contact processes** and Johann Wolfgang Döbereiner who spoke of **contact action** and whose lighter based on hydrogen and a platinum sponge became a huge commercial success in the 1820s. In the 1880s, Wilhelm Ostwald at Leipzig University started a series of systematic investigations into reactions that were catalyzed by the presence of acids and bases, and found both that chemical reactions occur at finite rates, and that these rates can be used to determine the strengths of acids and bases. For this work, Ostwald was awarded the 1909 Nobel Prize in Chemistry.*

History (wikipedia)

*The phrase catalysis was coined by Jöns Jakob Berzelius who in 1835 was the first to note that certain chemicals speed up a reaction. Other early chemists involved in catalysis were Alexander Mitscherlich who in 1831 referred to contact processes and Johann Wolfgang Döbereiner who spoke of contact action and whose lighter based on **hydrogen and a platinum sponge** became a huge commercial success in the 1820s. In the 1880s, Wilhelm Ostwald at Leipzig University started a series of systematic investigations into reactions that were catalyzed by the presence of acids and bases, and found both that chemical reactions occur at finite rates, and that these rates can be used to determine the strengths of acids and bases. For this work, Ostwald was awarded the 1909 Nobel Prize in Chemistry.*

History (wikipedia)

*The phrase catalysis was coined by Jöns Jakob Berzelius who in 1835 was the first to note that certain chemicals speed up a reaction. Other early chemists involved in catalysis were Alexander Mitscherlich who in 1831 referred to contact processes and Johann Wolfgang Döbereiner who spoke of contact action and whose lighter based on **hydrogen and a platinum sponge** became a huge commercial success in the 1820s. In the 1880s, Wilhelm Ostwald at Leipzig University started a series of systematic investigations into reactions that were catalyzed **by the presence of acids and bases**, and found both that chemical reactions occur at finite rates, and that these rates can be used to determine the strengths of acids and bases. For this work, Ostwald was awarded the 1909 Nobel Prize in Chemistry.*

History (wikipedia)

The phrase catalysis was coined by Jöns Jakob Berzelius who in 1835 was the first to note that certain chemicals speed up a reaction. Other early chemists involved in catalysis were Alexander Mitscherlich who in 1831 referred to contact processes and Johann Wolfgang Döbereiner who spoke of contact action and whose lighter based on hydrogen and a platinum sponge became a huge commercial success in the 1820s. In the 1880s, Wilhelm Ostwald at Leipzig University started a series of systematic investigations into reactions that were catalyzed by the presence of acids and bases, and found both that chemical reactions occur at finite rates, and that these rates can be used to determine the strengths of acids and bases. For this work, Ostwald was awarded the 1909 Nobel Prize in Chemistry.

Homogeneous or heterogeneous catalysis

Different **types of catalysts**:

Homogeneous catalysts catalyst, reactants and products in the same phase (e.g. all liquids).

Heterogeneous catalysts catalyst in a separate phase (e.g. solid catalyst of a gaseous reaction).

Obvious advantage of heterogeneous catalysts: the homogeneous catalysts needs to be removed after the reaction is performed!

Homogeneous or heterogeneous catalysis

Different **types of catalysts**:

Homogeneous catalysts catalyst, reactants and products in the **same phase** (e.g. all liquids).

Heterogeneous catalysts catalyst in a separate phase (e.g. solid catalyst of a gaseous reaction).

Obvious advantage of heterogeneous catalysts: the homogeneous catalysts needs to be removed after the reaction is performed!

Homogeneous or heterogeneous catalysis

Different **types of catalysts**:

Homogeneous catalysts catalyst, reactants and products in the **same phase** (e.g. all liquids).

Heterogeneous catalysts catalyst in a **separate phase** (e.g. solid catalyst of a gaseous reaction).

Obvious advantage of heterogeneous catalysts: the homogeneous catalysts needs to be removed after the reaction is performed!

Homogeneous or heterogeneous catalysis

Different types of catalysts:

Homogeneous catalysts catalyst, reactants and products in the same phase (e.g. all liquids).

Heterogeneous catalysts catalyst in a separate phase (e.g. solid catalyst of a gaseous reaction).

Obvious **advantage** of **heterogeneous catalysts**: the homogeneous catalysts needs to be removed after the reaction is performed!

Homogeneous or heterogeneous catalysis

Different types of catalysts:

Homogeneous catalysts catalyst, reactants and products in the same phase (e.g. all liquids).

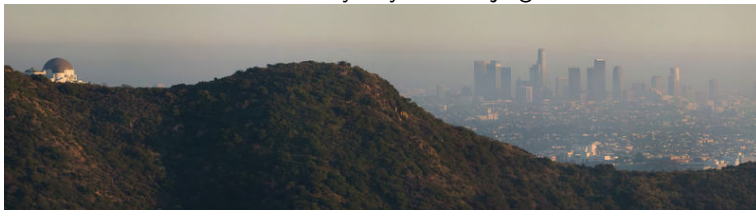
Heterogeneous catalysts catalyst in a separate phase (e.g. solid catalyst of a gaseous reaction).

Obvious advantage of heterogeneous catalysts: the **homogeneous catalysts** needs to be **removed** after the reaction is performed!

Real-world example



Two sunny days on Beijing



and Los Angeles

Car exhaust system. . .



Three main reactions are being catalysed at the same time

- ▶ $2\text{CO}_{(g)} + \text{O}_{2(g)} \rightarrow 2\text{CO}_{2(g)}$
- ▶ $2\text{NO}_{(g)} + 2\text{CO}_{(g)} \rightarrow \text{N}_{2(g)} + 2\text{CO}_{2(g)}$
- ▶ $\text{C}_6\text{H}_{6(g)} + 7\frac{1}{2}\text{O}_2 \rightarrow 6\text{CO}_{2(g)} + 3\text{H}_2\text{O}_{(l)}$

Car exhaust system. . .

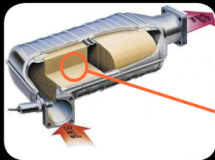


Three main reactions are being catalysed at the same time

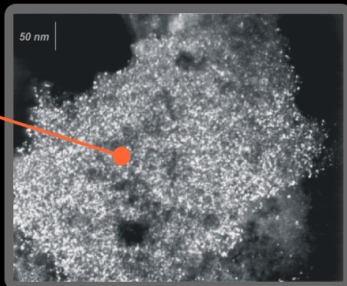
- ▶ $2\text{CO}_{(g)} + \text{O}_{2(g)} \rightarrow 2\text{CO}_{2(g)}$
- ▶ $2\text{NO}_{(g)} + 2\text{CO}_{(g)} \rightarrow \text{N}_{2(g)} + 2\text{CO}_{2(g)}$
- ▶ $\text{C}_6\text{H}_{6(g)} + 7\frac{1}{2}\text{O}_2 \rightarrow 6\text{CO}_{2(g)} + 3\text{H}_2\text{O}_{(l)}$

... and the catalyst itself

Real catalyst

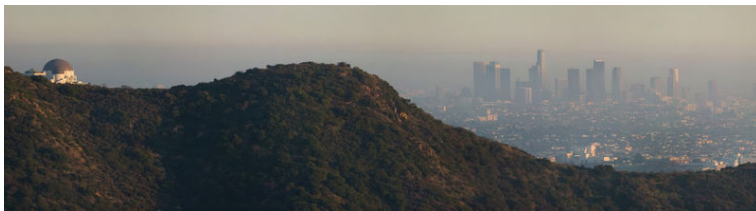


eg: 3-way car
exhaust system



$\text{Pd}/(\text{Ce}, \text{Zr})\text{O}_x/\text{Al}_2\text{O}_3$, Martinez-Arias et al., *J. Catal.* 204, 292 (2001)

Ingeneering

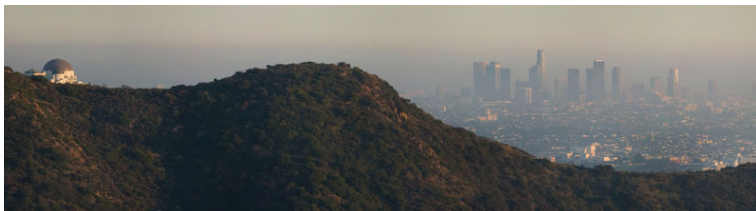


Do you want to **improve** its **performance**?

Typically, heterogeneous catalysis is a complex process

1. take an old one
2. change a few of its properties
3. try the new catalyst
4. try 100+ new catalysts
5. sell the best one

Ingeneering

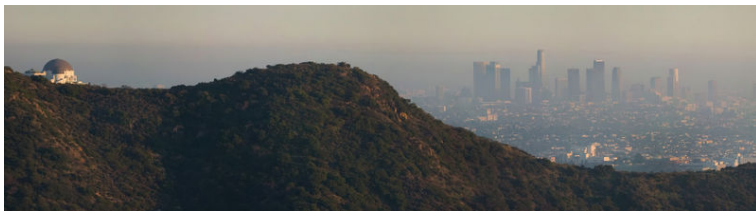


Do you want to improve its performance?

Typically, heterogeneous catalysis is a **complex process**

1. take an old one
2. change a few of its properties
3. try the new catalyst
4. try 100+ new catalysts
5. sell the best one

Ingeneering

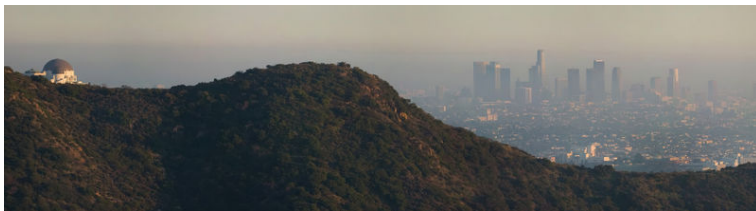


Do you want to improve its performance?

Typically, heterogeneous catalysis is a **complex process**

1. take an old one
2. change a few of its properties
3. try the new catalyst
4. try 100+ new catalysts
5. sell the best one

Ingeneering

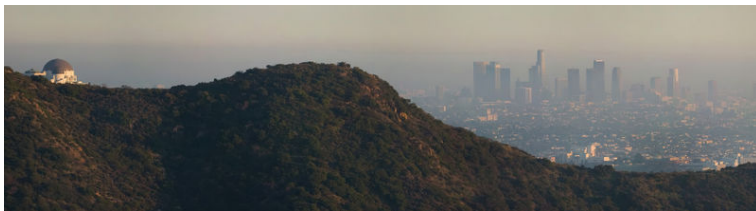


Do you want to improve its performance?

Typically, heterogeneous catalysis is a **complex process**

1. take an old one
2. change a few of its properties
3. try the new catalyst
4. try 100+ new catalysts
5. sell the best one

Ingeneering

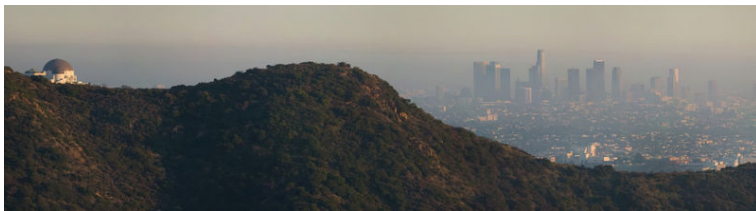


Do you want to improve its performance?

Typically, heterogeneous catalysis is a **complex process**

1. take an old one
2. change a few of its properties
3. try the new catalyst
4. try 100+ new catalysts
5. sell the best one

Ingeneering

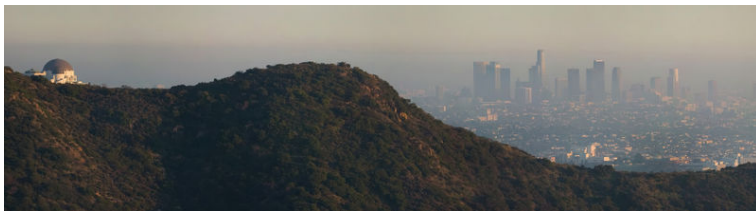


Do you want to improve its performance?

Typically, heterogeneous catalysis is a **complex process**

1. take an old one
2. change a few of its properties
3. try the new catalyst
4. try 100+ new catalysts
5. sell the best one

Ingeneering

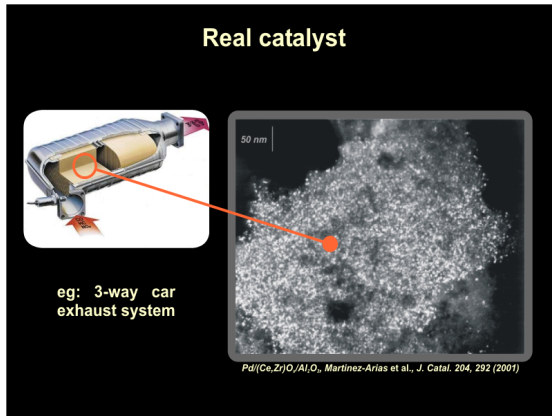


Do you want to improve its performance?

Typically, heterogeneous catalysis is a **complex process**

1. take an old one
2. change a few of its properties
3. try the new catalyst
4. try 100+ new catalysts
5. sell the best one

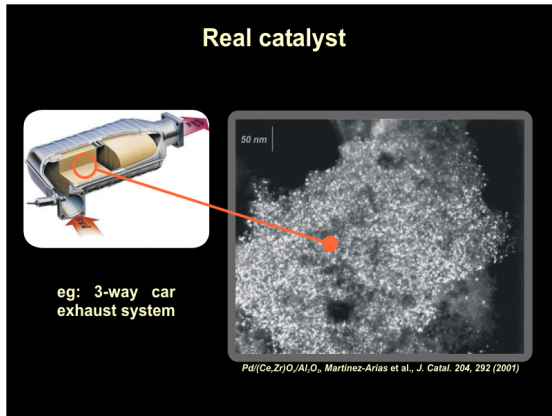
Conclusion



And what if...

... we could understand what happens at this surface?

Conclusion



And what if...

... we could **understand** what happens at this surface?

Outline

Introduction

Catalysis

What is catalysis?

Homogeneous or heterogeneous catalysis

Example of heterogeneous catalysis

Ingeneering?

Surface Science

Complex surfaces

Complex reactions at complex surfaces

Intelligent materials

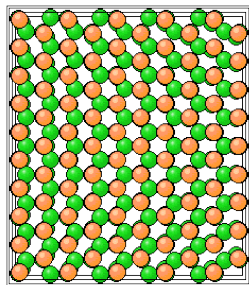
Windows

Nanotechnologies

Studying surfaces

Because not only the chemical reactions are complex but the surface itself is!

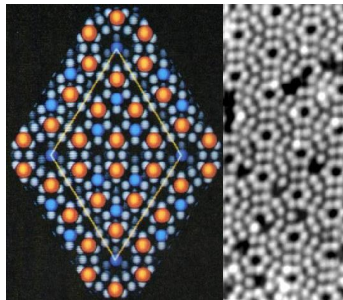
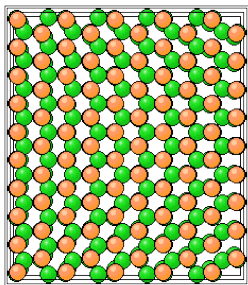
(e.g. Si)



Studying surfaces

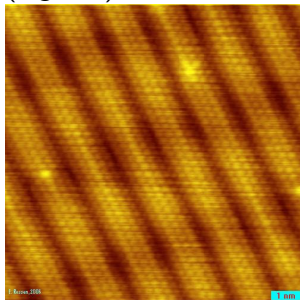
Because not only the chemical reactions are complex but the surface itself is!

(e.g. Si)



Complex surfaces

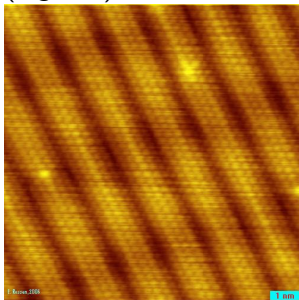
(e.g. Au)



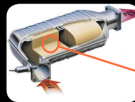
Very simple surfaces and realistic surfaces!

Complex surfaces

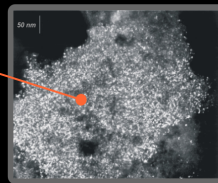
(e.g. Au)



Real catalyst



eg: 3-way car
exhaust system



Pd[(Ce,Zr)O/Al₂O₃], Martínez-Arias et al., J. Catal. 204, 292 (2001)

Very simple surfaces and **realistic surfaces**!

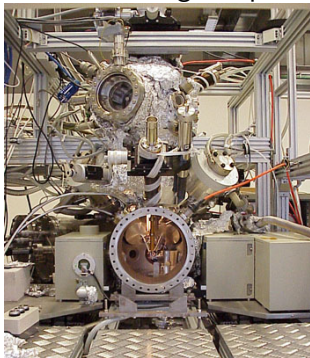
Studying complex reactions at complex surfaces?

... or breaking the problem into pieces

Work under vacuum, use simpler surfaces with known properties,
and simple reaction...

Studying complex reactions at complex surfaces?

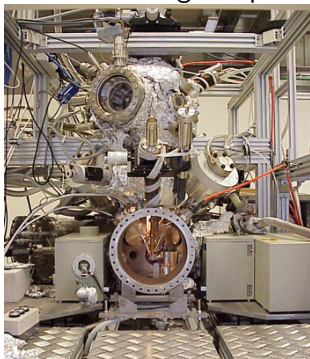
... or breaking the problem into pieces



Work under **vacuum**, use simpler surfaces with known properties,
and simple reaction. . .

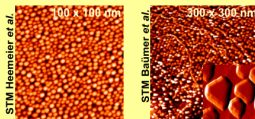
Studying complex reactions at complex surfaces?

... or breaking the problem into pieces



Model Catalysts

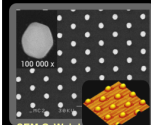
$\text{Pd}/\text{Al}_2\text{O}_3/\text{NiAl}(110)$ - prepared *in situ*



Pd at./island	100	2700
Surface Pd atoms	60	540
Island size	$1.8 \pm 0.4 \text{ nm}$	$5.5 \pm 0.7 \text{ nm}$

Catal. Lett. 71, 5 (2001)

EBL prepared
 Pd/SiO_2
from Göteborg, Sweden



SEM G. Weinberg
AFM Ann Grant

Diameter: 500 nm
Height: 450 nm

J. Catal. 201, 275 (2001)

Work under vacuum, use **simpler surfaces** with **known properties**,
and simple reaction...

Outline

Introduction

Catalysis

What is catalysis?

Homogeneous or heterogeneous catalysis

Example of heterogeneous catalysis

Ingeneering?

Surface Science

Complex surfaces

Complex reactions at complex surfaces

Intelligent materials

Windows

Nanotechnologies

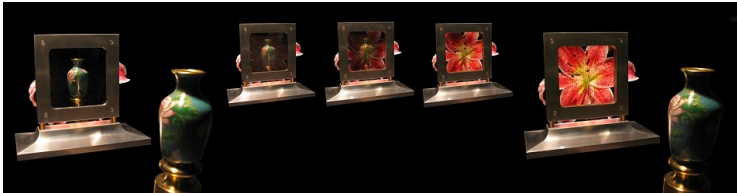
Self-cleaning materials



A window covered with an invisible coating of catalyzer which destroys the organic dirt as it is deposited.

from St. Gobain

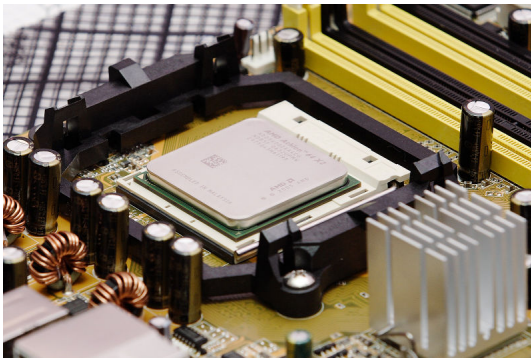
Energy savings



Mirror or window?

from the Windows and Daylighting Group at Lawrence Berkeley National Lab.

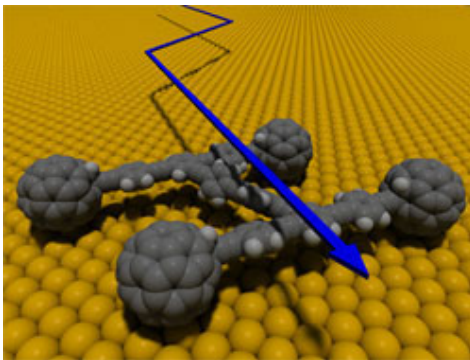
CPU chip



CPU chip layout based on surface science

AMD X2 3600

The nanocar



Prof. James Tour's nanocar, Rice University

Acknowledgements

- ▶ Fritz-Haber-Institut, F. A. Universität
 - ▶ Prof. Dr. Libuda
 - ▶ Prof. Dr. Dr. Freund
 - ▶ A. Desikusumastuti
- ▶ The University of Tokyo
 - ▶ Dr. H. Kondoh
 - ▶ H. Ariga, R. Kohda, J. Fujimori
- ▶ Japanese Society for the Promotion of Science and the Science dialogue program
- ▶ Tsuru High School, Yamanashi prefecture and Ms. M. Komiya
- ▶ Wikipedia (most of the pictures in this presentation)