2245-26

Joint ICTP-IAEA Advanced School on the Role of Nuclear Technology in Hydrogen-Based Energy Systems

13 - 18 June 2011

Computational modeling of catalytic materials for H2-based technologies

Stefano Fabris

CNR-IOM Democritos Center
Trieste

Computational modeling of catalytic materials for H_2-based technologies

Stefano Fabris

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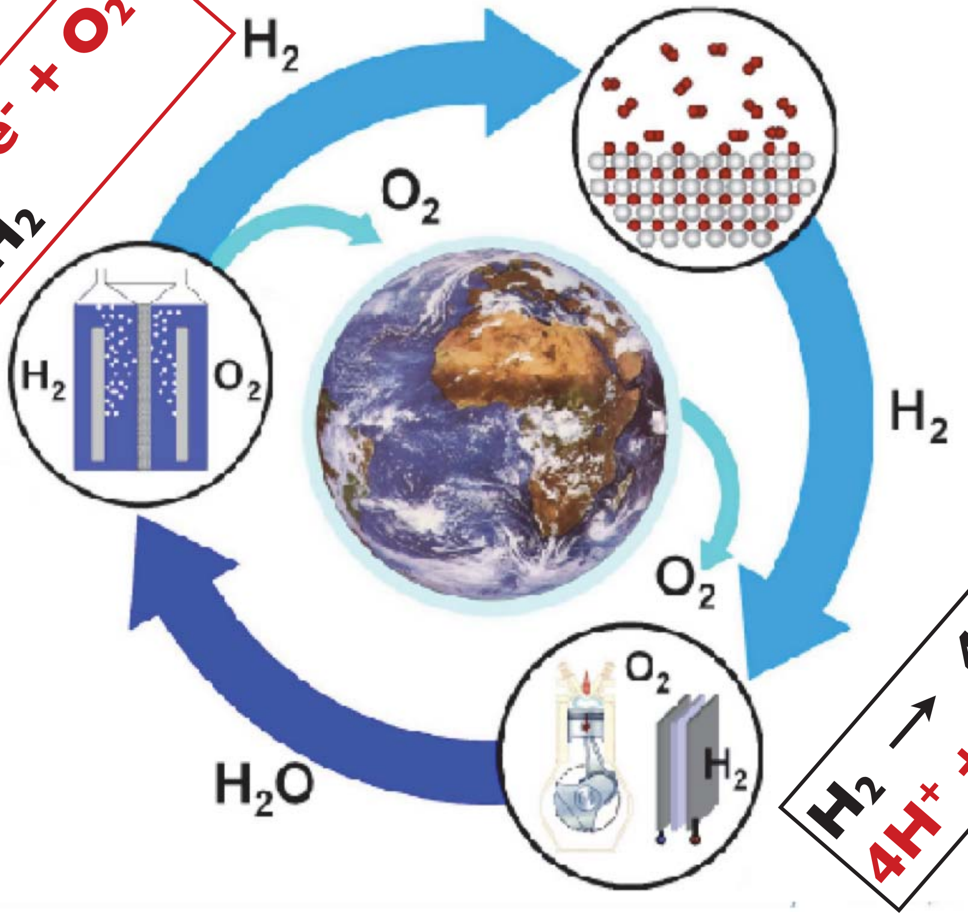
SISSA - Scuola Internazionale Superiore di Studi Avanzati
Trieste - ITALY

Catalysis in the H2-cycle

The sustainable production and usage of fuels relies on (electro)chemical reactions

$2H_2O \rightarrow 4H^+ + 4e^- + O_2$

$4H^+ + 4e^- \rightarrow H_2$



$H_2 \rightarrow 4H^+ + 4e^-$

$4H^+ + 4e^- + O_2 \rightarrow 2H_2O$

These electrochemical reactions are thermodynamically and kinetically demanding: requires efficient and stable CATALYST (possibly cheap)

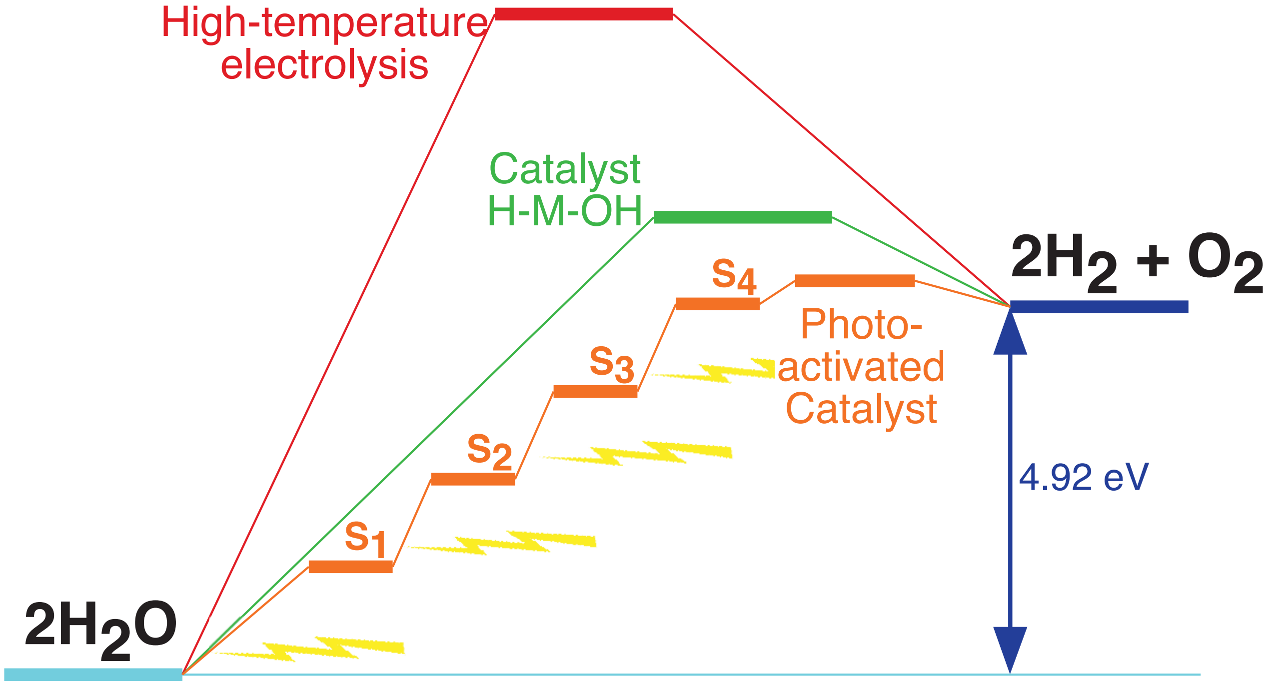
Example: water oxidation

$2H_2O \rightarrow 4H^+ + 4e^- + O_2$

$4H^+ + 4e^- \rightarrow H_2$

- ✳Thermodynamically very endothermic - DG=4.92 eV, E0=1.23 V
- ✳Formidable complexity at molecular level:

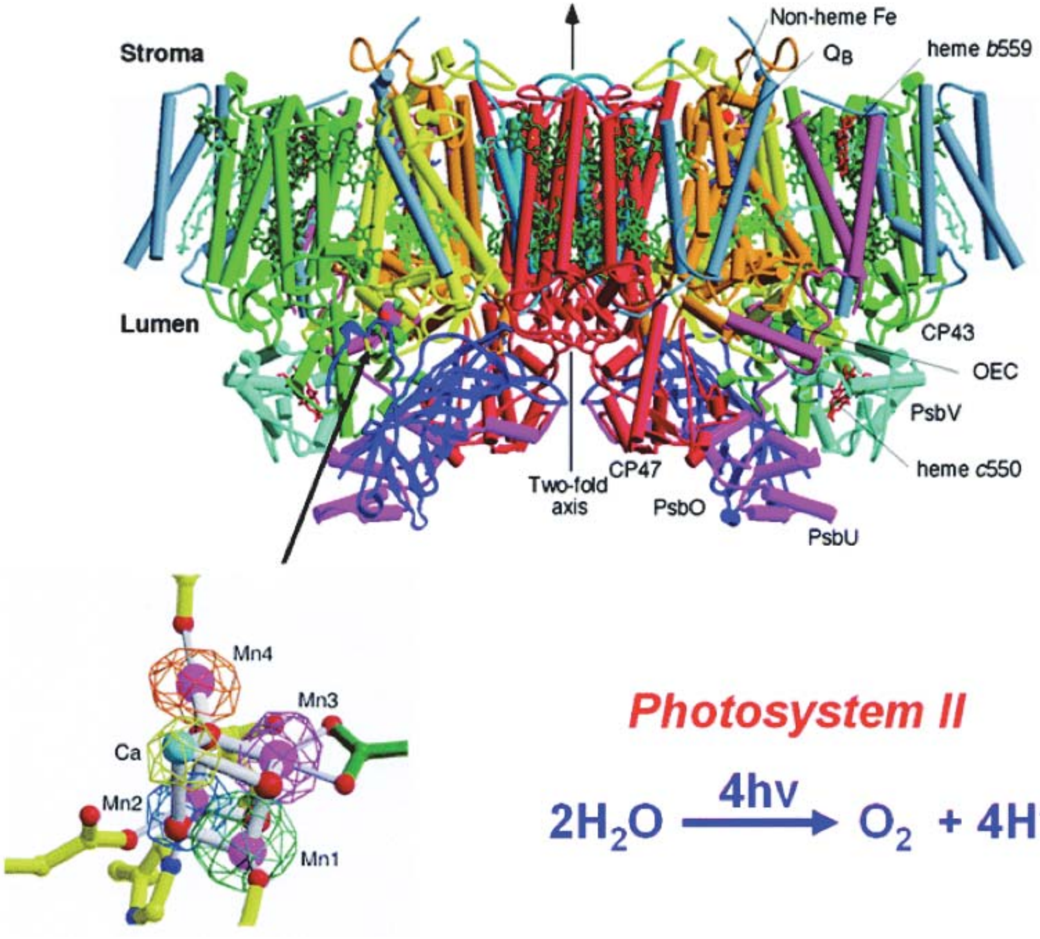
  removal of 4 protons and 4 electrons from 2 water molecules + O2 formation



A catalyst is required to minimize the activation barrier and to maximize the rate

Finding new catalysts

Nature, in billions of years, developed a multicenter metal-oxo core catalyst



Photosystem II

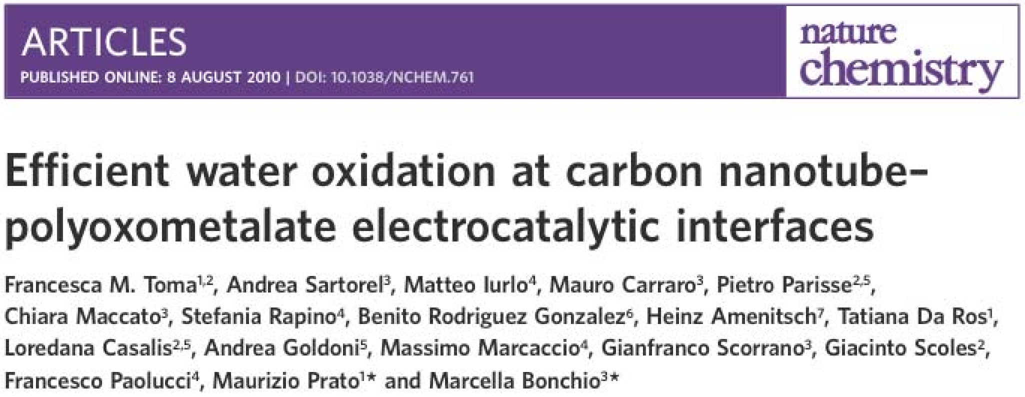
$$2H_2O \xrightarrow{4hv} O_2 + 4H^+ + 4e$$

Materials science challenge

Design artificial catalysts which are highly efficient, stable and based on earth abundant elements

Finding new catalysts

Recent synthesis of many promising systems …



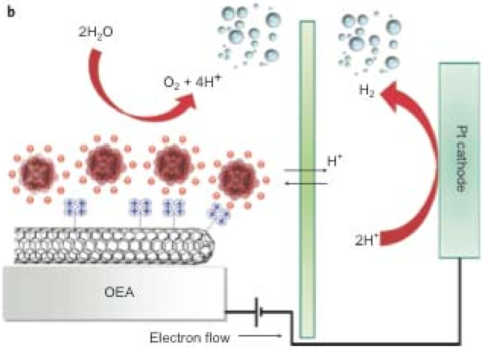
ARTICLES

PUBLISHED ONLINE: 8 AUGUST 2010 | DOI: 10.1038/NCHEM.761

nature chemistry

Efficient water oxidation at carbon nanotube–polyoxometalate electrocatalytic interfaces

Francesca M. Toma[1,2], Andrea Sartorel[3], Matteo Iurlo[4], Mauro Carraro[3], Pietro Parisse[2,5], Chiara Maccato[3], Stefania Rapino[4], Benito Rodriguez Gonzalez[6], Heinz Amenitsch[7], Tatiana Da Ros[1], Loredana Casalis[2,5], Andrea Goldoni[5], Massimo Marcaccio[4], Gianfranco Scorrano[3], Giacinto Scoles[2], Francesco Paolucci[4], Maurizio Prato[1]* and Marcella Bonchio[3]*



In Situ Formation of an Oxygen-Evolving Catalyst in Neutral Water Containing Phosphate and Co^{2+}

Matthew W. Kanan and Daniel G. Nocera*

Science
AAAS

…

What is the fundamental origin of their efficiency?
Which are the mechanisms at the basis of their functions?
What can be modified to improve performances or discover new systems?

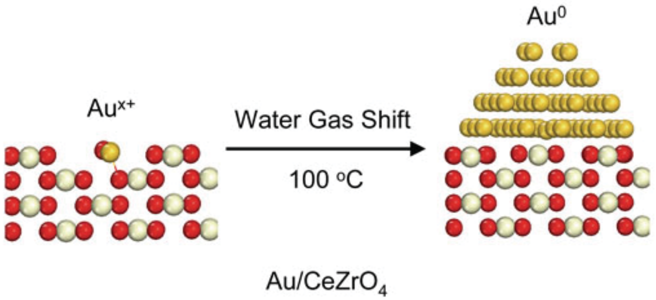
Role of materials modeling

To provide insight into these fundamental issues and identify guidelines

Finding new catalysts

… for H2 production and purification from hydrocarbons

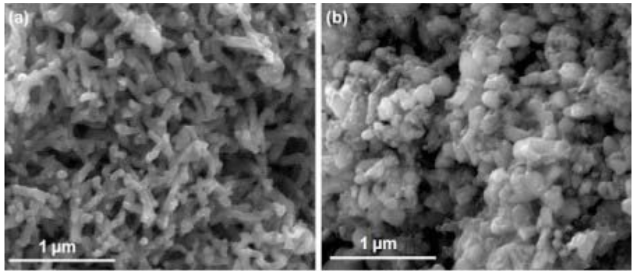
(steam reforming, water-gas-shift, preferential oxidation, …)

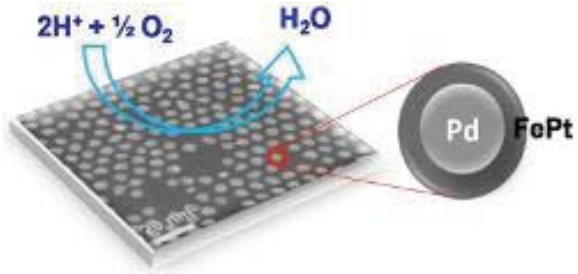


Steam reforming	$CH_4 + H_2O \rightarrow CO + 3H_2$
Water Gas Shift	$CO + H_2O \rightarrow CO_2 + H_2$
Preferential oxidation	$2CO + O_2 \rightarrow 2CO_2$

… for efficient H2 utilization in fuel cells

$$\mathbf{H_2 \rightarrow 4H^+ + 4e^-}$$
$$\mathbf{4H^+ + 4e^- + O_2 \rightarrow 2H_2O}$$

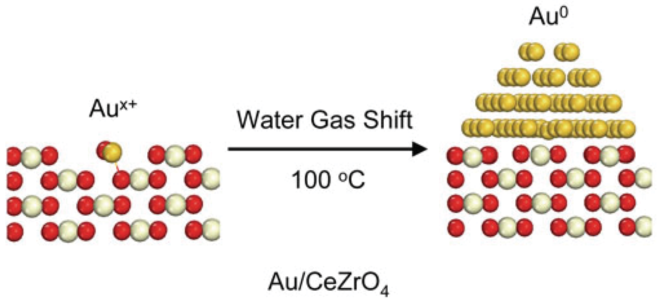




Finding new catalysts

... for H2 production and purification from hydr ons

(steam reforming, water-gas-shift, preferential oxid)



Steam reforming $H_2O \rightarrow CO + 3H_2$

Water Gas Shift $O + H_2O \rightarrow CO_2 + H_2$

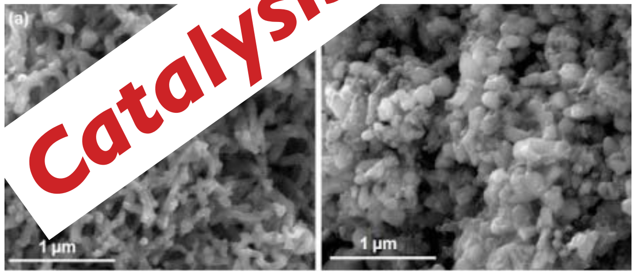
Preferential $2CO + O_2 \rightarrow 2CO_2$

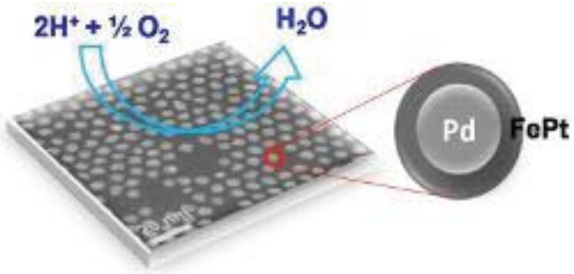
... for effici utilization in fuel cells

$\rightarrow 4H^+ + 4e^-$

$H^+ + 4e^- + O_2 \rightarrow 2H_2O$

Catalysis is a key issue in H2-based technologies

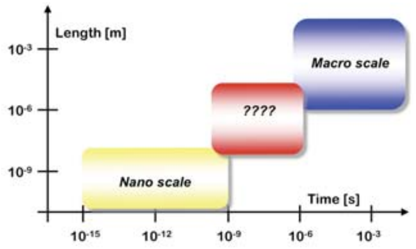




Outline

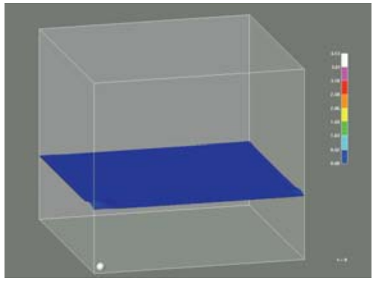
Role and expected outcome of numerical modeling

time and length scales: importance of sub-micron scale
levels of theory & accuracy
general remarks



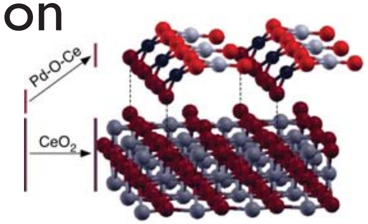
Computational techniques

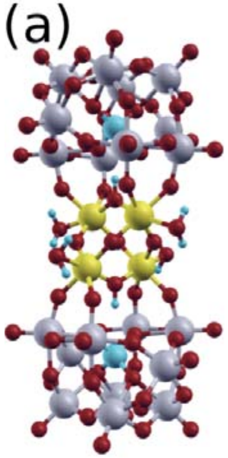
Density Functional Theory
Intermolecular forces and Molecular Dynamics
QM/MM approaches
Simulating chemical reactions and rare events
Ab-initio thermodynamics and effect of chemical environment



Working cases

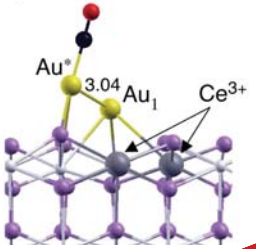
Homogeneous metal-organic molecular catalysts
Multicenter metal-oxo cores for H2 production
Oxide-supported metal nanoparticles
Design of new electrodes for fuel cells

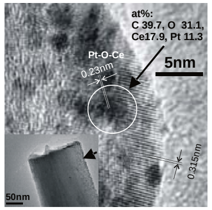


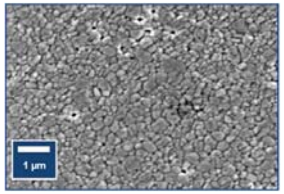


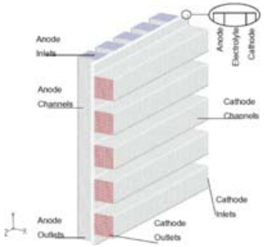
Time and Length scales

Design and operation of H_2-based technologies









10^{-10} m

10^{-9} m

10^{-6} m

10^{-1} m

1 m

10^{1} m

11 orders of magnitude in length scales
17 orders of magnitude in time scales

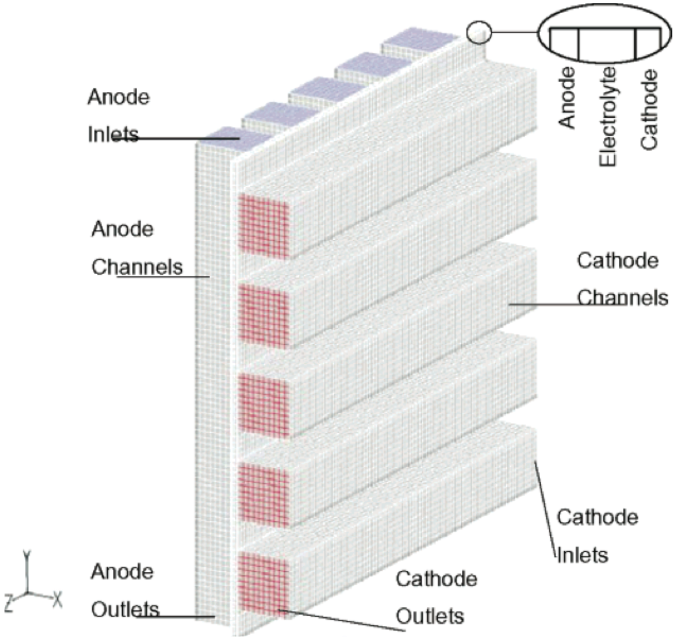
Natural divide at around 10^{-6} m

Macro and homogeneous scales

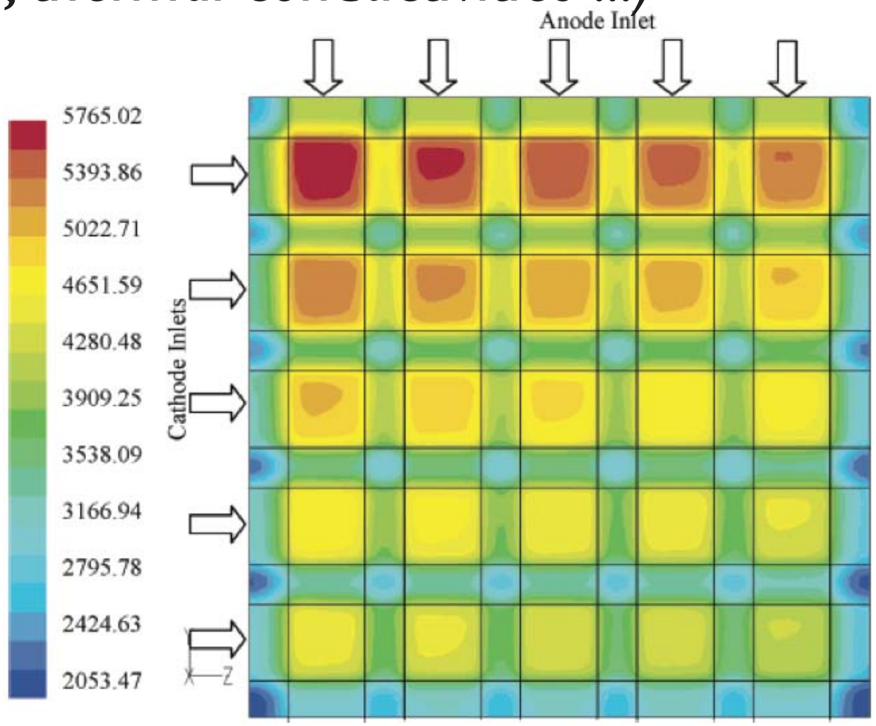
$L > 10^{-6}$ m

The system can be modeled as a continuum in terms of effective properties

(transport coefficients, thermal conductivities ...)



SOFC



Simulated current distribution(A/m2)

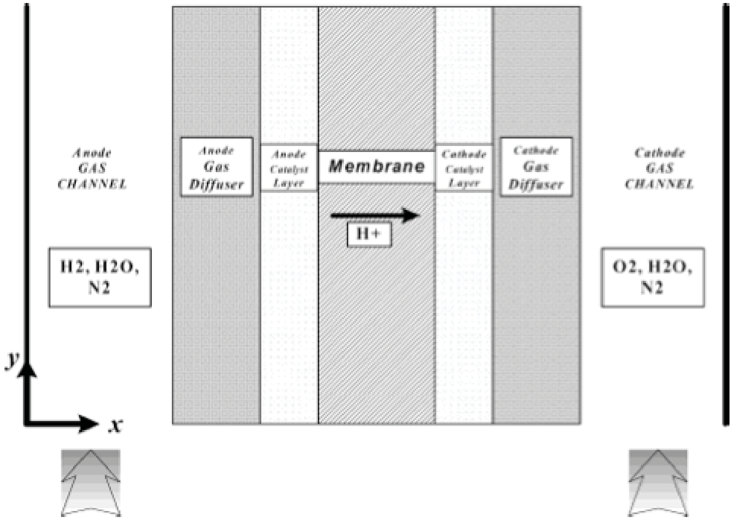
Device models at these scales

used to predict overall performance on the basis of averaged parameters

Macro and homogeneous

L> 10^{-6} m

Numerical modeling at this scale involves solving systems of equations for electrodes, membrane, flow fields ...



mass	$\partial(\epsilon\rho)/\partial t + \nabla(\rho\vec{u}) = S_m$
momentum	$1/\epsilon[\partial(\rho\vec{u})/\partial t + 1/\epsilon\nabla(\rho\vec{u}\vec{u})] = -\nabla p + \nabla\tau + S_u \quad S_u = (-\mu/K)\vec{u}$
species	$\partial(\epsilon C_k)/\partial t + \nabla(\vec{u}C_k) = \nabla(D_k{}^{\mathrm{eff}}\nabla C_k) + S_k$
charge	$\nabla(\kappa^{\mathrm{eff}}\nabla\Phi_e) + S_\Phi = 0$
	$\nabla(\sigma^{\mathrm{eff}}\nabla\Phi_s) - S_\Phi = 0$
energy	$\partial[(\rho c_{\mathrm{p}})_m T]/\partial t + \nabla(\rho c_{\mathrm{p}}\vec{u}T) = \nabla(k^{\mathrm{eff}}\nabla T) + S_T$

Prediction of overall performance on the basis
of averaged parameters:
flow field patterns, AC impedence, ...

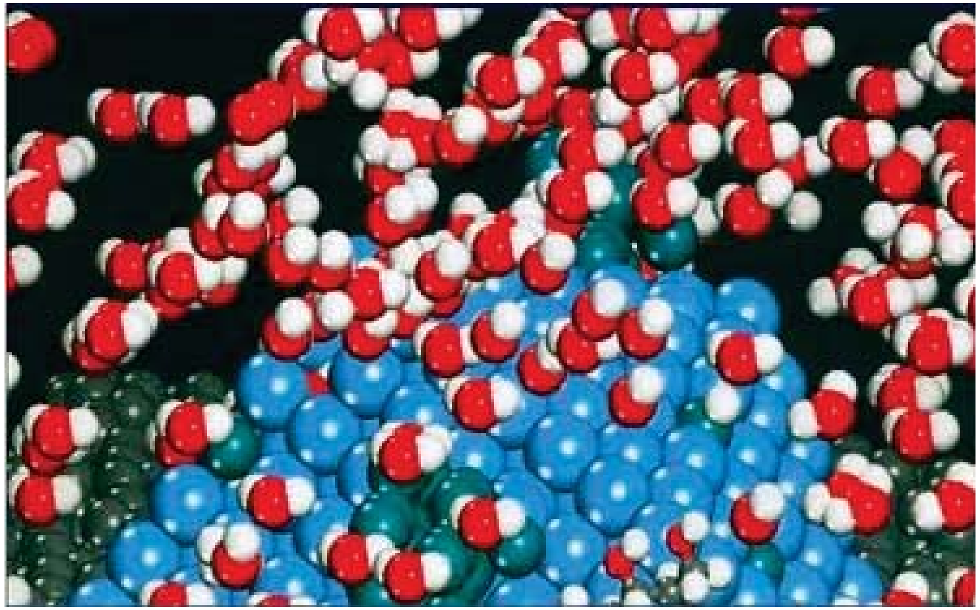
Device models at these scales

cannot explain how to find/design new materials with the desired parameters!

Sub-micron scale: materials modeling

The system is modeled describing explicitly its atomistic nature

(crystalline/polycrystalline/amorphous structure, interfaces, ...)



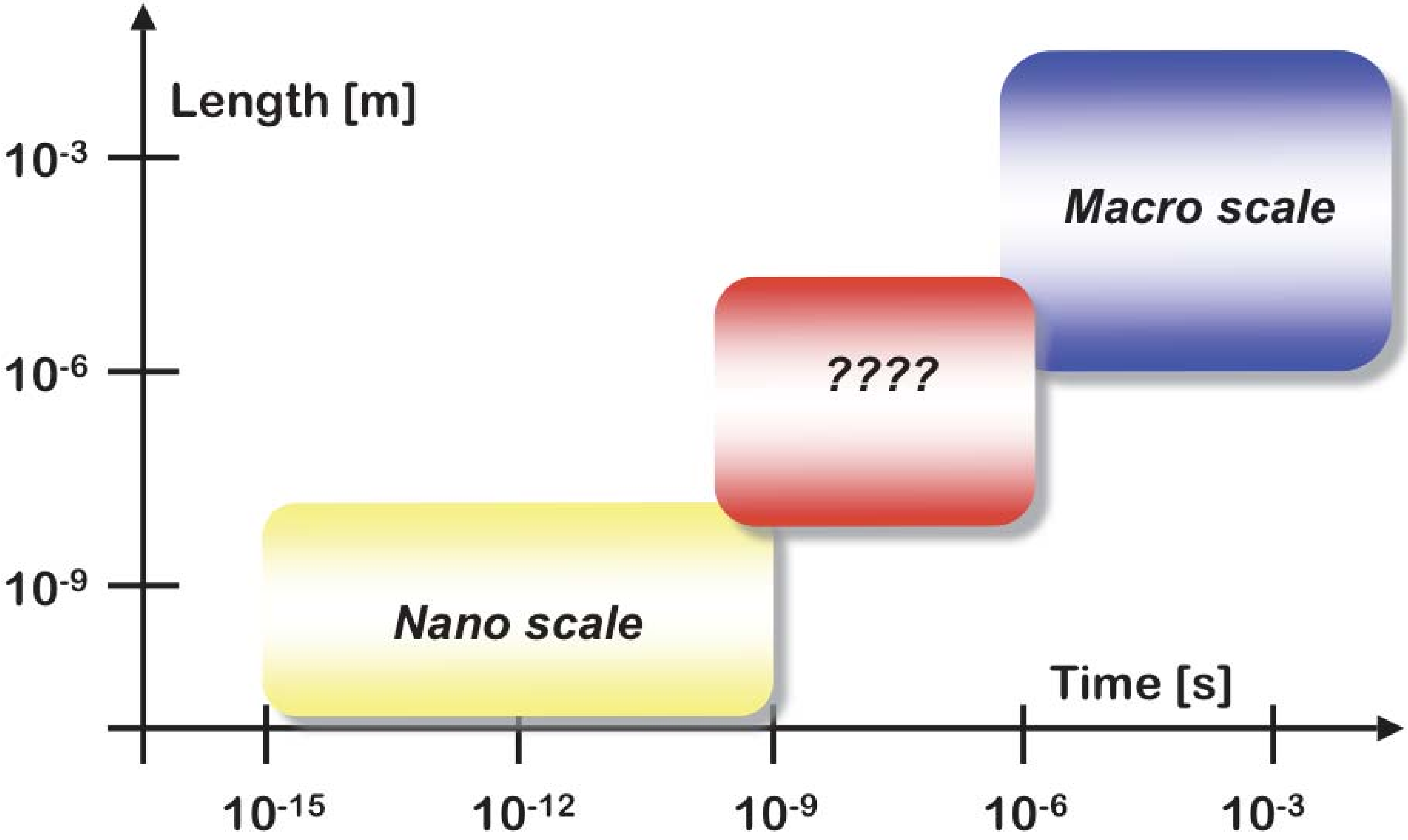
Fuel cell catalysts: a surface science approach
(M. Koper)

The role of materials modeling is two fold:

- to elucidate the mechanisms behind the averaged properties of the super-micron scales

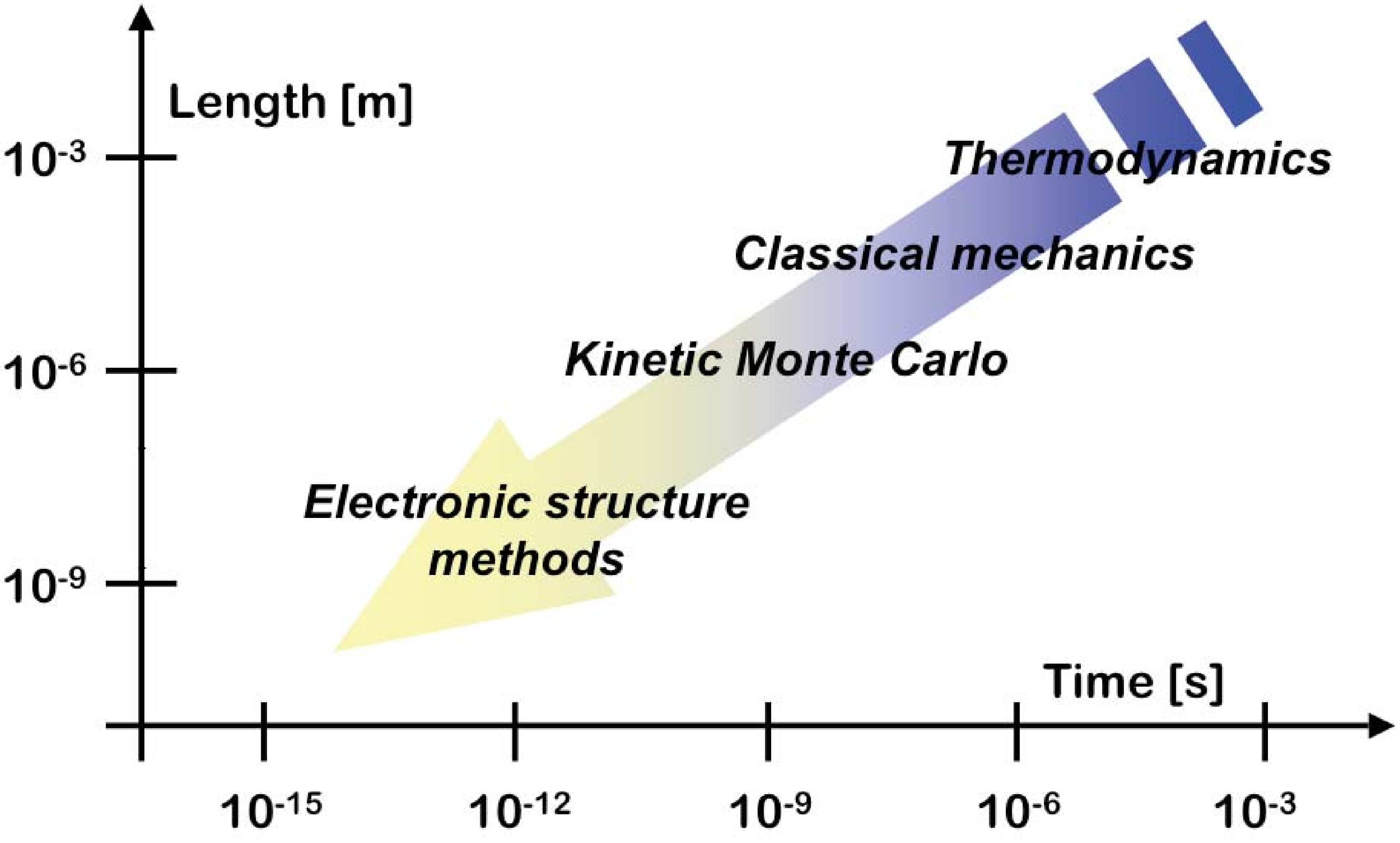
- to provide insight for
  - ➡rational design of novel materials/systems
  - ➡incremental improvement of existing materials/systems

Time and length scales

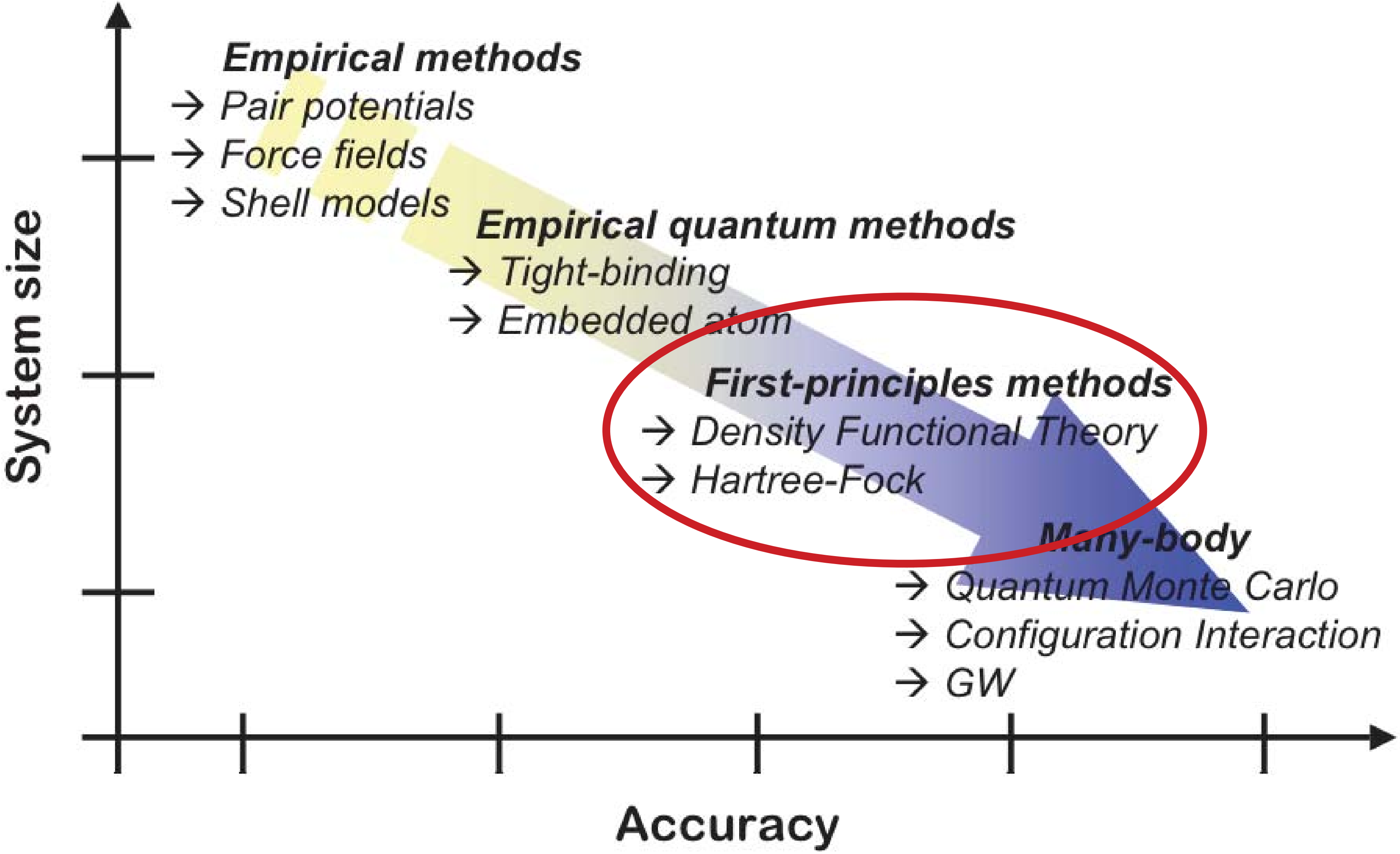


We have currently little ideas on how to model efficiently the scales between the nanometer-micron ones

Time and length scales



Methods and approximations



The lecture focuses on materials modeling based on quantum mechanics

good compromise between predictive power and accuracy

DFT-based materials modeling

High-quality packages are available

Appealing to non-specialists, *easy* to use, often *free*:

are becoming very popular

www.quantum-espresso.org ... *and many others*

but beware:

false impression that these simulations requires *just* solving the basic equations of quantum mechanics

The Rubbish-in Rubbish-out risk

“Accurate and predictive materials modeling requires

THEORIES APPROXIMATIONS ALGORITHMS

all of them has to be validated and used correctly”

Only then one can aim at giving useful insight into materials property (not only fuel cells or H2-based technologies)

Materials modeling implies a MODEL

Devising a “model” is crucial and requires great care

What is a useful model?

“It allow to isolate elements of the complex physics that regulate the system and to understand the contributions of different factors”

REMARK 1: this is almost impossible to achieve with experiments

What is the important outcome?

“The most important outcome of computational materials modeling is INSIGHT into the fundamental phenomena occurring in the system”

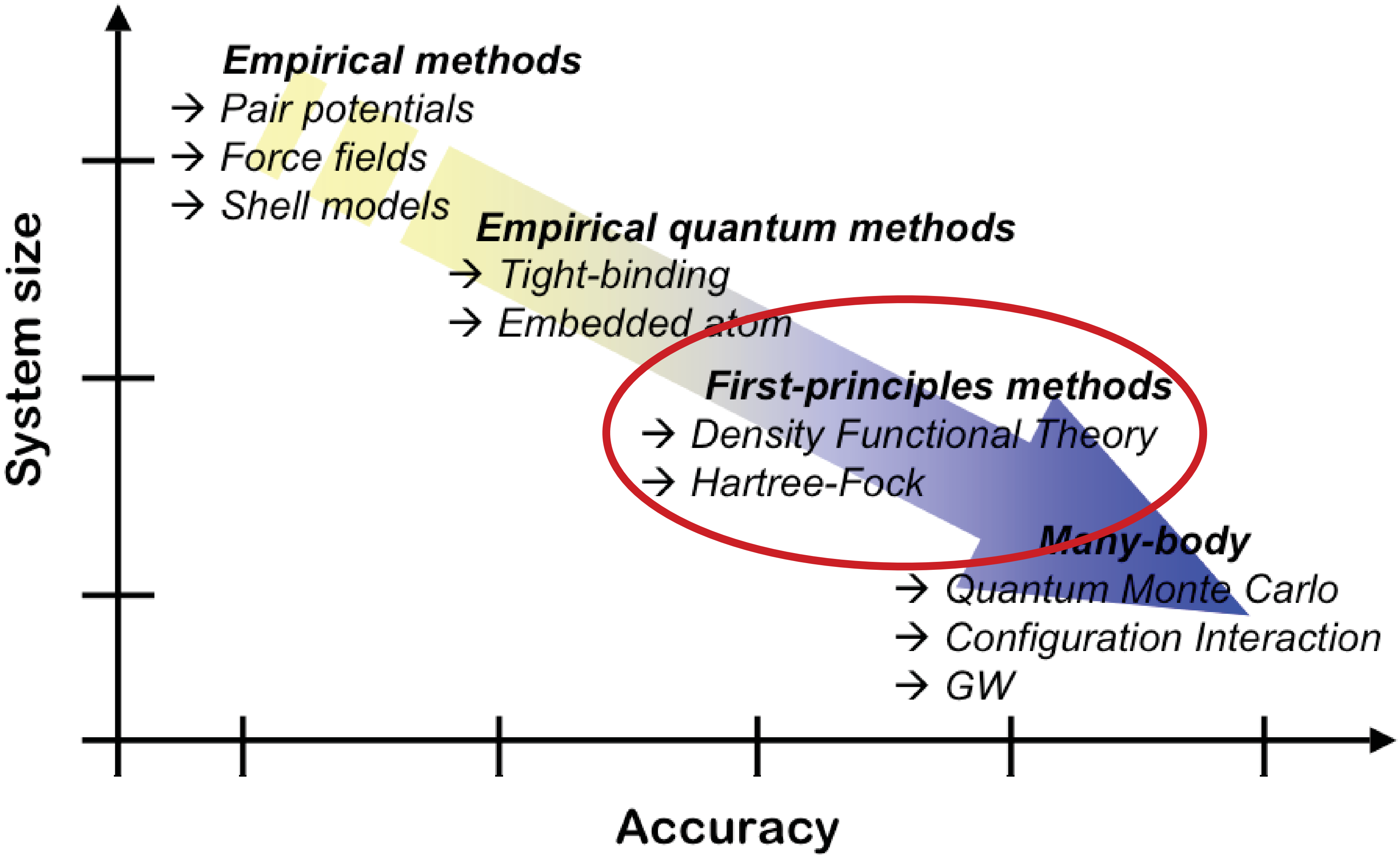
REMARK 2: a model is not reality

Model validation: contact with experiment

“The next-important thing to consider in computational modeling is the VALIDATION of the model and of the predictions”

REMARK 3: contact/feedback with experiment is crucial

Methods and approximations



Empirical methods

→ *Pair potentials*
→ *Force fields*
→ *Shell models*

Empirical quantum methods

→ *Tight-binding*
→ *Embedded atom*

First-principles methods

→ *Density Functional Theory*
→ *Hartree-Fock*

Many-body

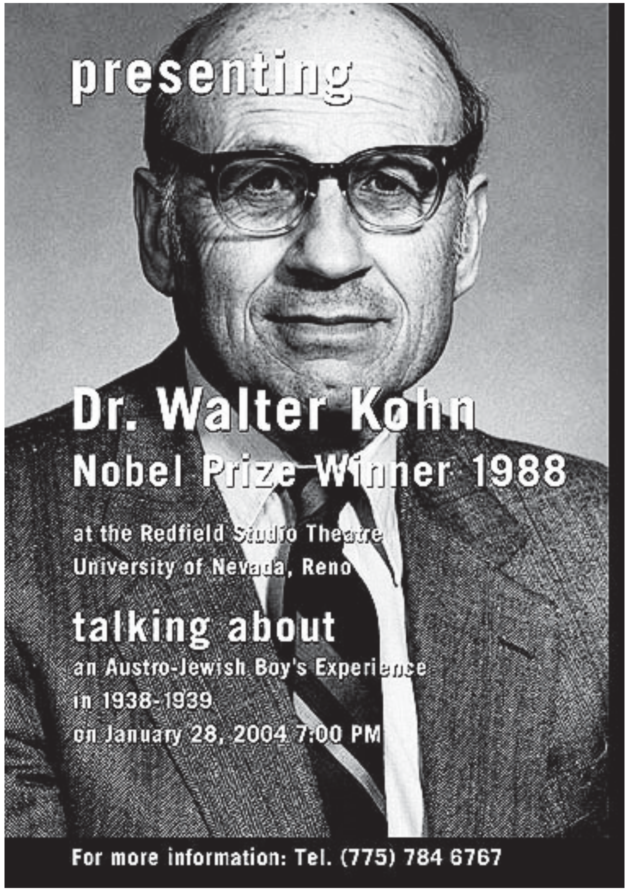
→ *Quantum Monte Carlo*
→ *Configuration Interaction*
→ *GW*

The lecture focuses on materials modeling based on quantum mechanics

Density Functional Theory

P. Hohenberg and W. Kohn. Phys. Rev. 136, 864 (1964)
W. Kohn and L. J. Sham. Phys. Rev. 140, 1133 (1965)

DFT is now a well established method for calculating



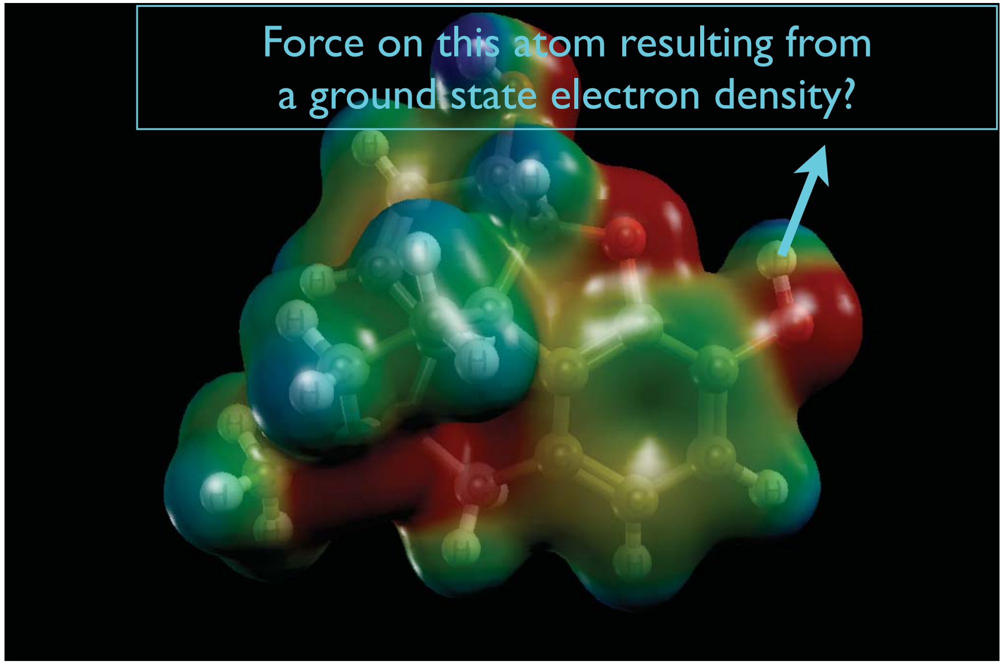
- Ground-state charge density ⬅
- Band structure
- Total energy (differences) ⬅
- Atomic forces ⬅
- Structural optimization
- Lattice dynamics and phonons
- Molecular dynamics ⬅
- Optical properties
- ...

Limitations
Strong electron correlations
Van der Waals
...

... of systems with up to some hundreds of independent atoms

Ab-initio interatomic forces

From the charge density to interatomic forces



Force on this atom resulting from a ground state electron density?

Hellmann-Feynman theorem

Energy variations are second order in the electron density

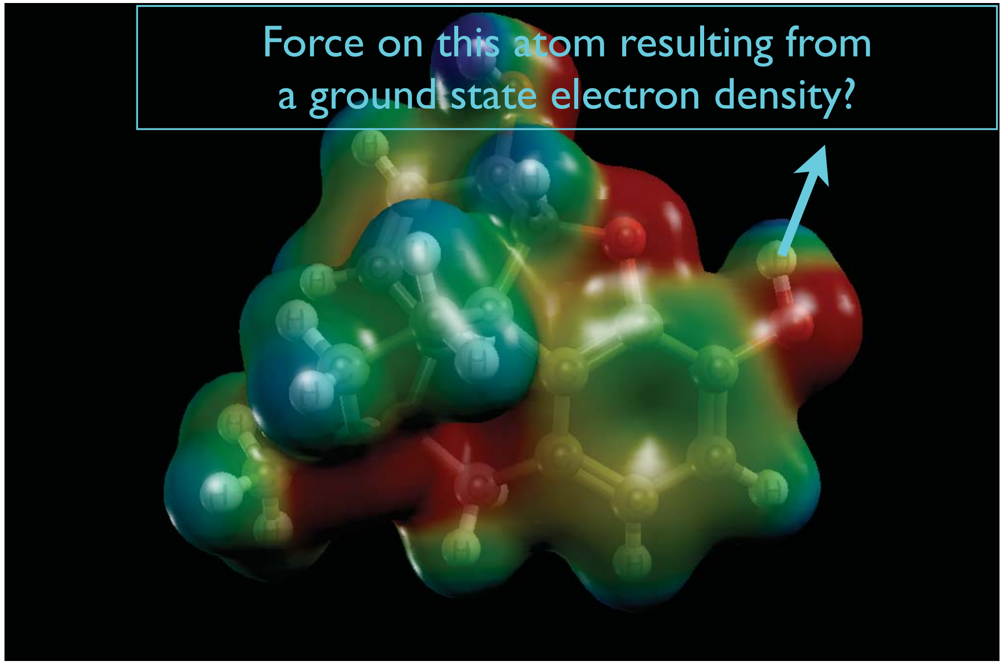
$$\mathbf{F}_I = -\frac{\partial E}{\partial \mathbf{R}_I} = \left\langle \Psi_{\mathbf{R}} \middle| \frac{\partial H}{\partial \mathbf{R}_I} \middle| \Psi_{\mathbf{R}} \right\rangle$$

Interatomic forces can be calculated on the basis of the ground state density only

!STRAIGHTFORWARD!

Ab-initio interatomic forces

From the charge density to interatomic forces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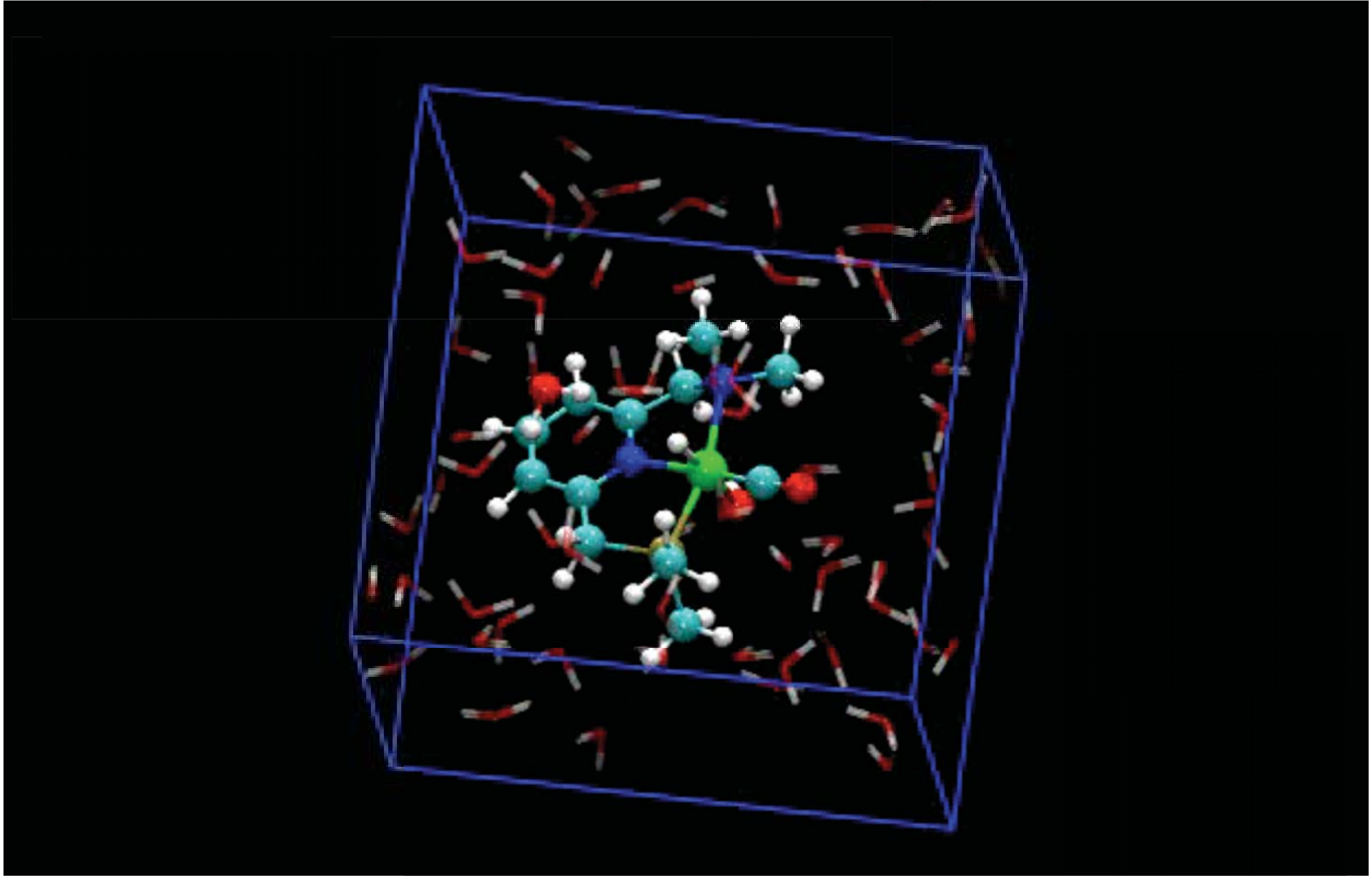
From interatomic forces to molecular dynamics

$$M_I \ddot{\mathbf{R}}_I = \mathbf{F}_I$$

Numerical integration of the equations of motion

Compute equilibrium and transport properties of classical many-body systems

Ab-initio molecular dynamics



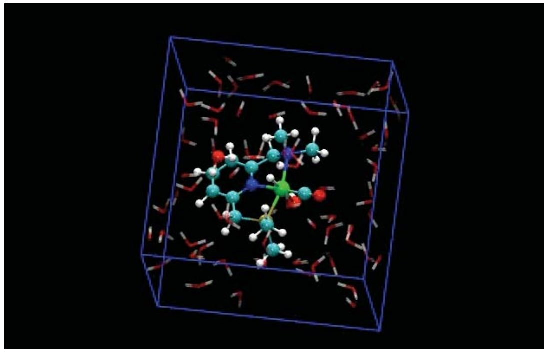
C. Ma, S. Piccinin, and SF, in preparation

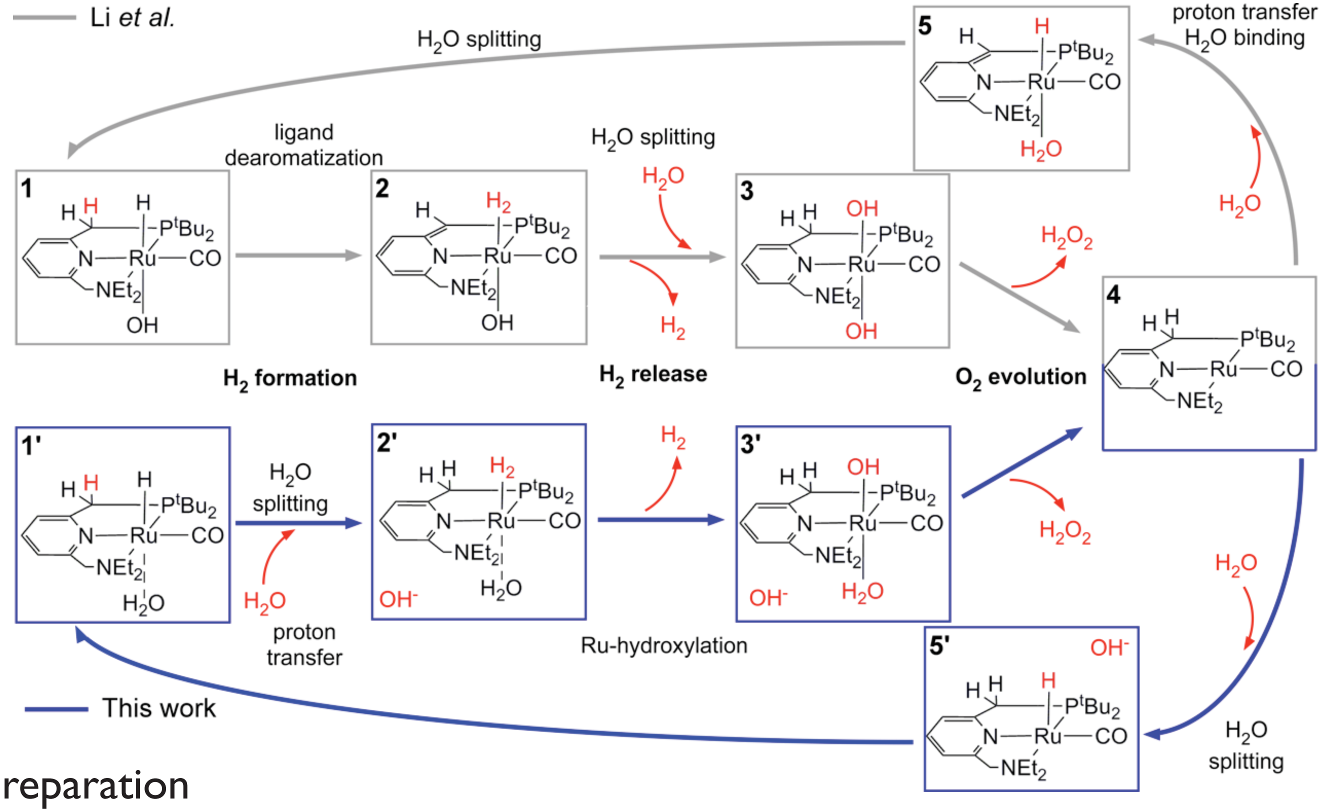
Ab-initio molecular dynamics

3 APRIL 2009 VOL 324 SCIENCE

Consecutive Thermal H_2 and Light-Induced O_2 Evolution from Water Promoted by a Metal Complex

Stephan W. Kohl,[1] Lev Weiner,[2] Leonid Schwartsburd,[1] Leonid Konstantinovski,[2] Linda J. W. Shimon,[2] Yehoshoa Ben-David,[1] Mark A. Iron,[2] David Milstein[1]*





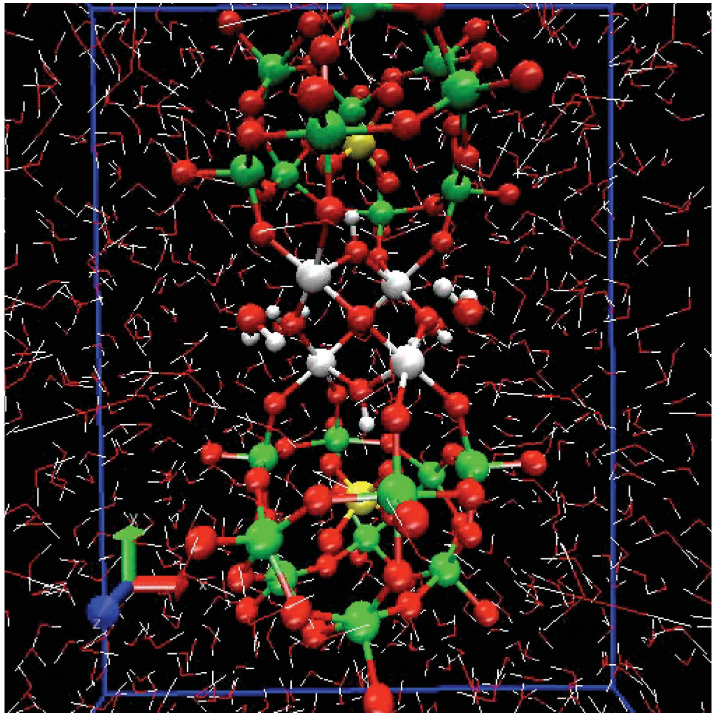
C. Ma, S. Piccinin, and SF, in preparation

Bridging length scales: QM/MM

Partition the system in two regions

Reaction region - QM

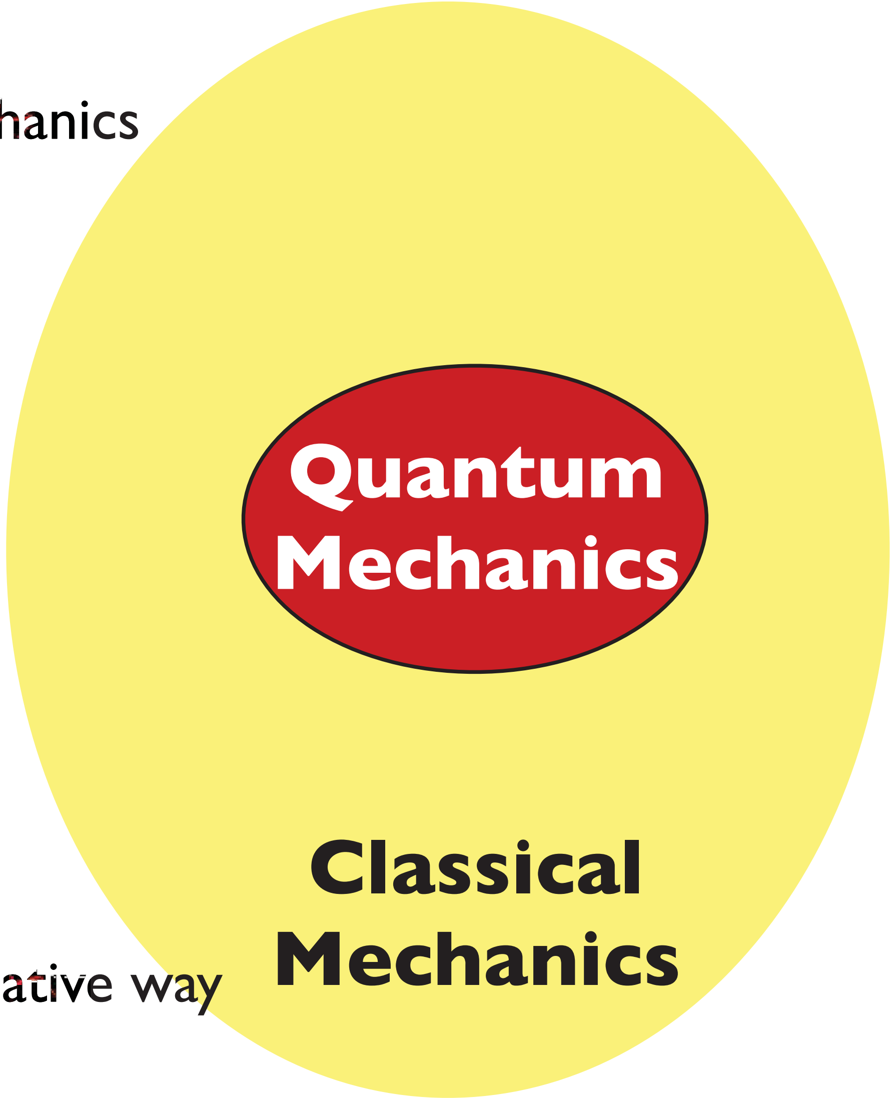
described at the level of Quantum Mechanics



Embedding region - MM

acts on the reaction center in a perturbative way

described by a classical force field



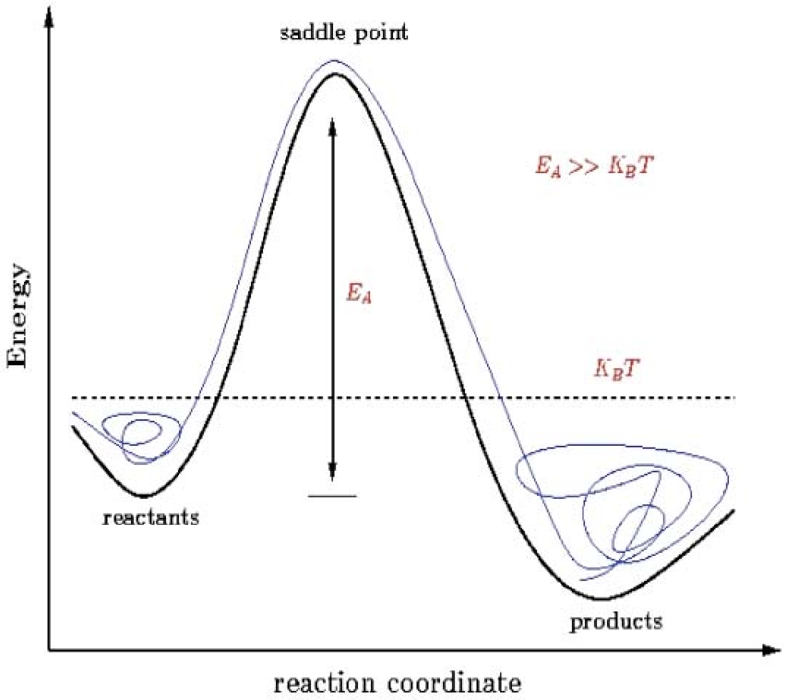
Simulating chemical reactions

Simulating rare (activated) events is challenging!

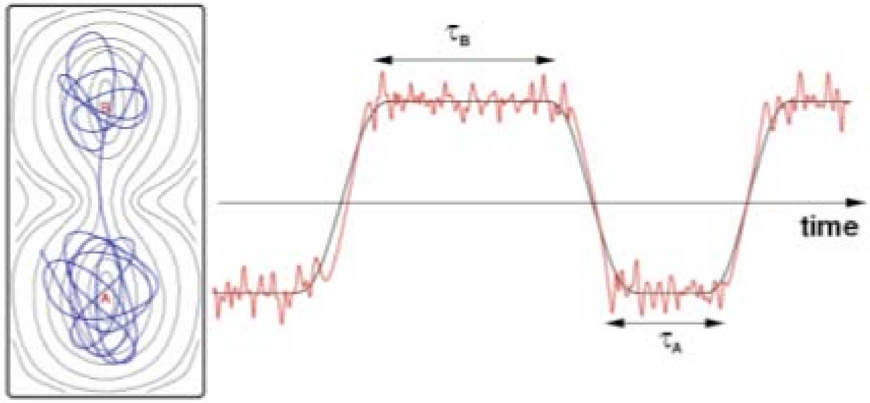
... beyond Molecular Dynamics

Steam reforming	$CH_4 + H_2O \rightarrow CO + 3H_2$
Water Gas Shift	$CO + H_2O \rightarrow CO_2 + H_2$
Preferential oxidation	$2CO + O_2 \rightarrow 2CO_2$

Reaction rates often not compatible with MD time-scales



$$k_{\text{reactants}\rightarrow\text{products}} = \mathcal{A} \cdot e^{-\frac{E_A}{K_B T}}$$



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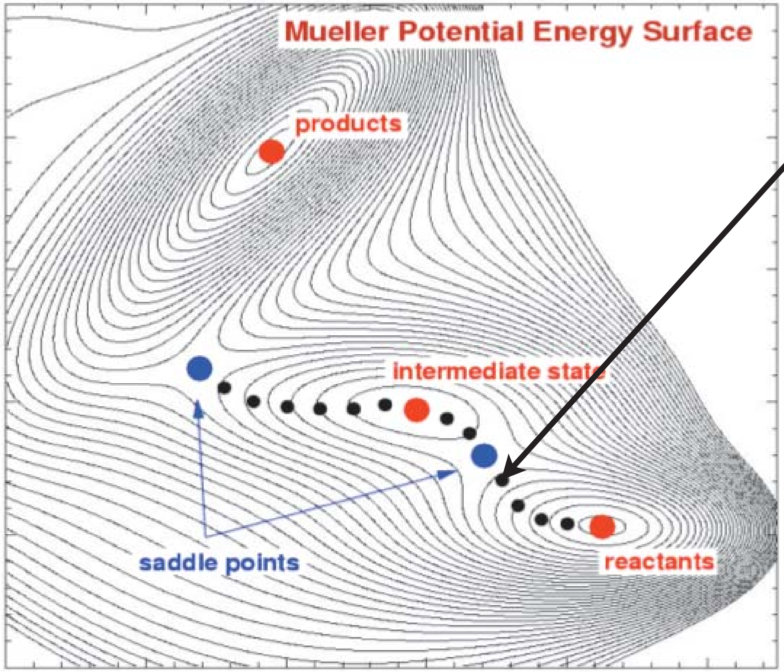
Simulation techniques for finding ***MINIMUM ENERGY PATH***

(ex: Nudged Elastic Band method)



path in the energy landscape having the highest probability of transition

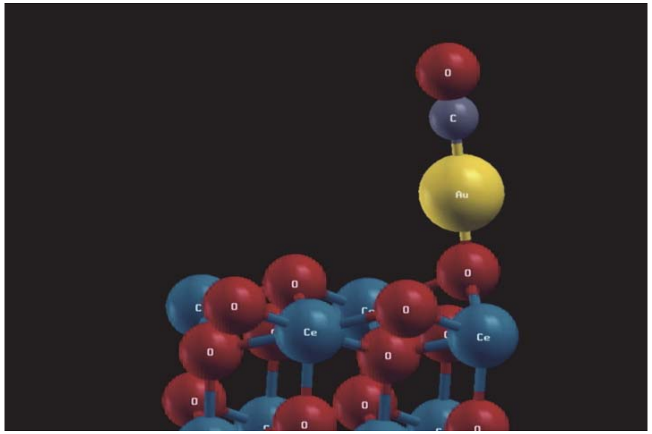
Outcome

- reaction mechanism
- reaction intermediates
- rate-limiting step
- activation energy

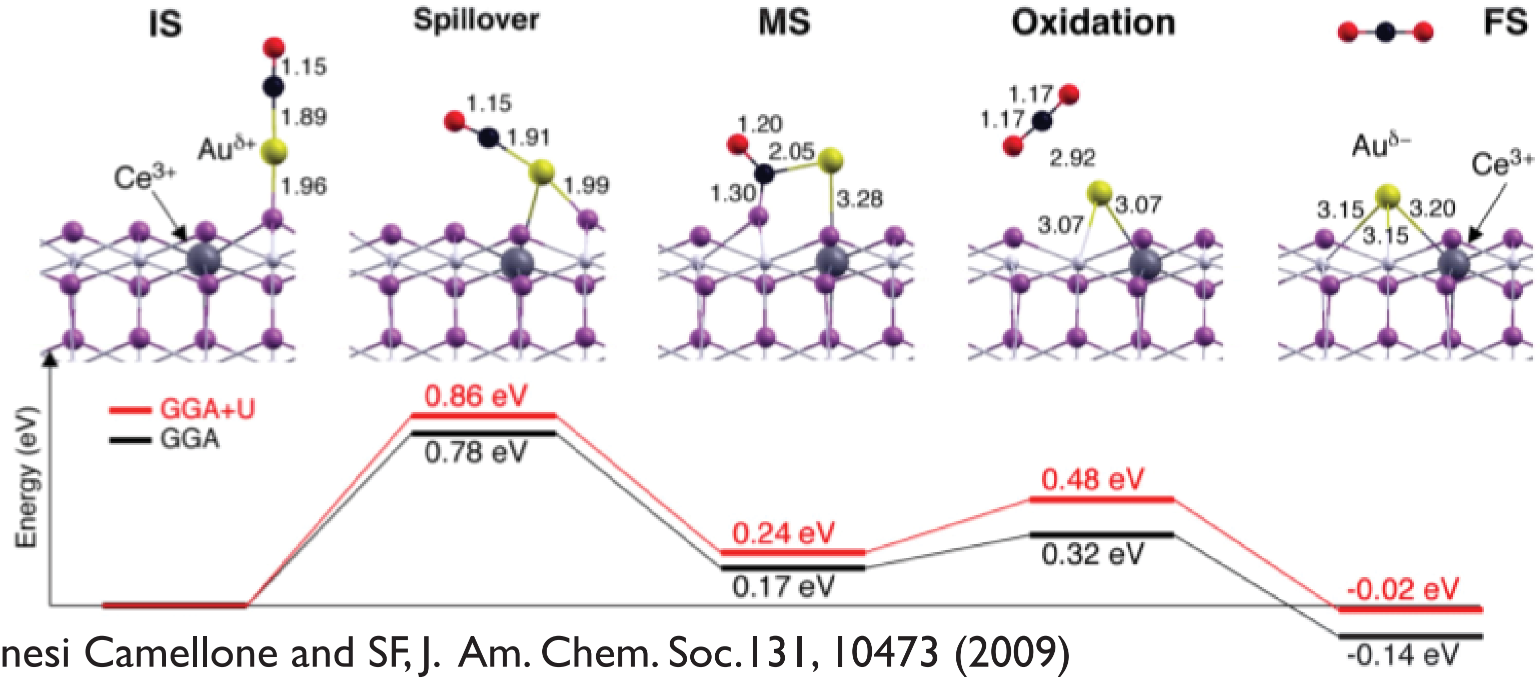
Preferential CO oxidation

$$2CO + O_2 \longrightarrow 2CO_2$$

catalyzed by metal nanoparticles
supported by reducible catalysts



Au/CeO2 catalysts
active role of the substrate as O buffer



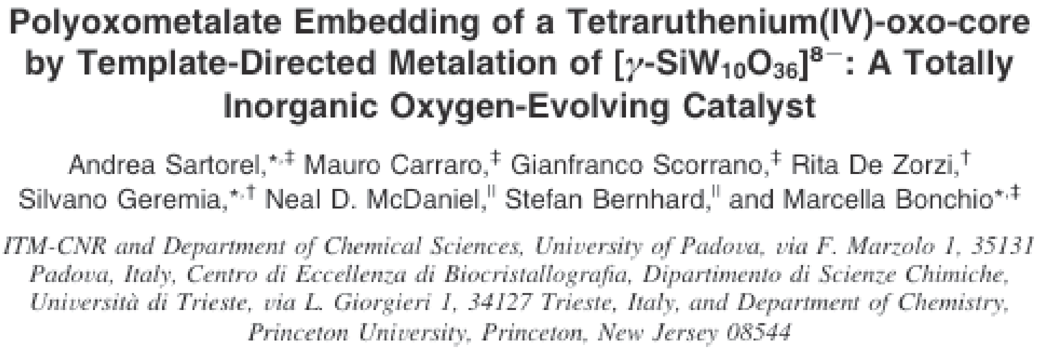
M. Farnesi Camellone and SF, J. Am. Chem. Soc.131, 10473 (2009)

Metadynamics

Simulating rare (activated) events without knowledge of the final state is even more challenging!

Ex: the formation of the O-O bond during water oxidation

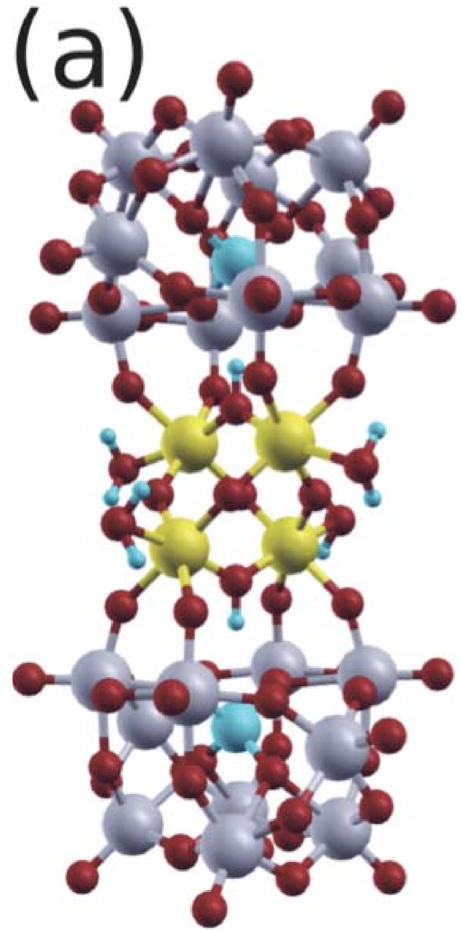
$$2H_2O \rightarrow 4H^+ + 4e^- + O_2$$
$$4H^+ + 4e^- \rightarrow H_2$$



Polyoxometalate Embedding of a Tetraruthenium(IV)-oxo-core by Template-Directed Metalation of $[\gamma\text{-SiW}_{10}O_{36}]^{8-}$: A Totally Inorganic Oxygen-Evolving Catalyst

Andrea Sartorel,*,‡ Mauro Carraro,‡ Gianfranco Scorrano,‡ Rita De Zorzi,†
Silvano Geremia,*,† Neal D. McDaniel,‖ Stefan Bernhard,‖ and Marcella Bonchio*,‡

ITM-CNR and Department of Chemical Sciences, University of Padova, via F. Marzolo 1, 35131 Padova, Italy, Centro di Eccellenza di Biocristallografia, Dipartimento di Scienze Chimiche, Università di Trieste, via L. Giorgieri 1, 34127 Trieste, Italy, and Department of Chemistry, Princeton University, Princeton, New Jersey 08544



One of the most efficient and stable catalysts reported so far

Working mechanism? Relevant intermediates?

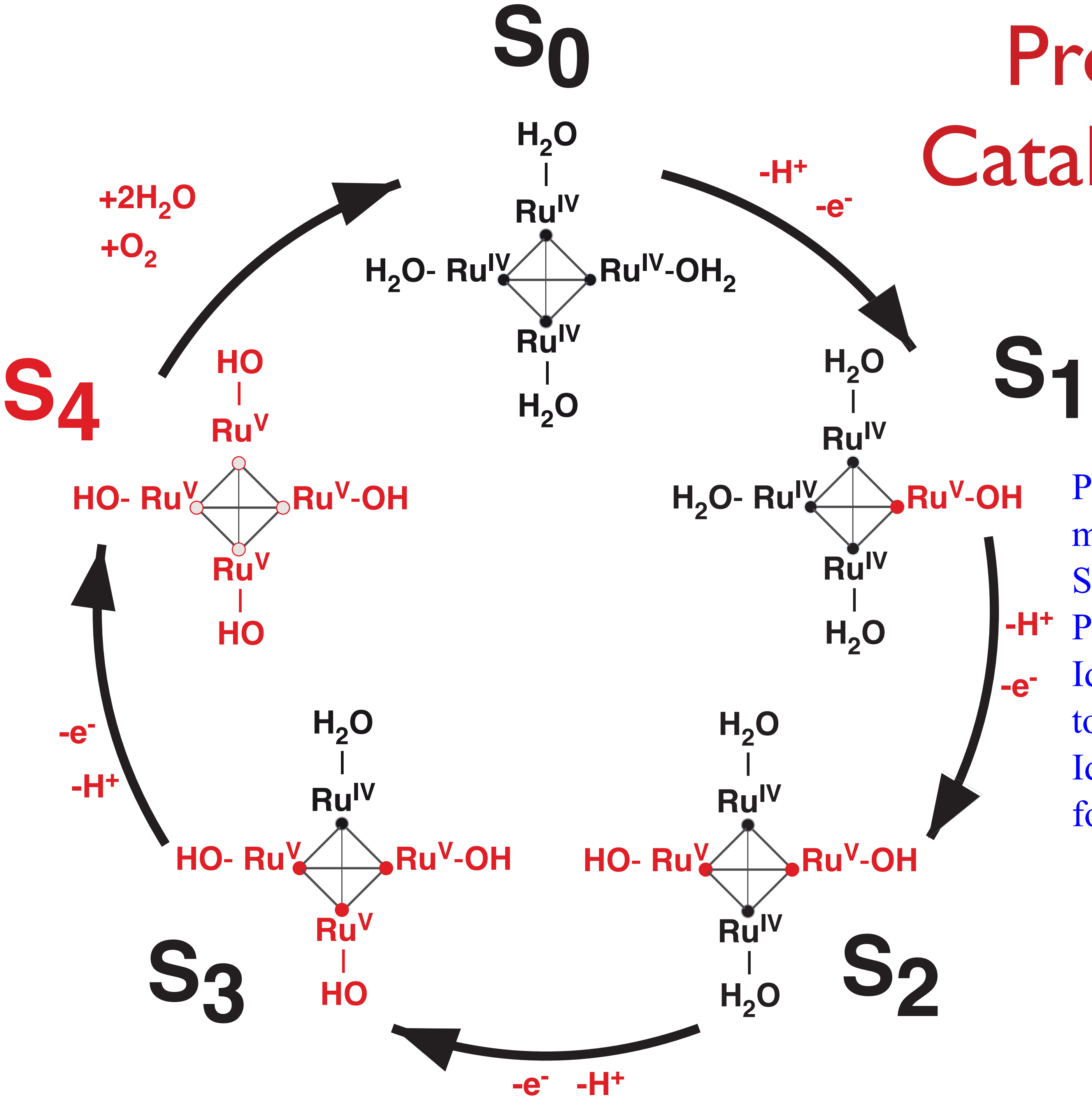
How does water split and an O2 molecule form?

Which are the thermodynamic and kinetic origin of this high efficiency and stability?

Is it possible to improve them? How?

Sartorel et al. JACS 130, 5006 (2008)
Geletii et al. Angew. Chem. Int. Ed. 47, 3896 (2008)

Proposed Catalytic cycle



GOALS

Provide insight into the working mechanisms of this catalyst

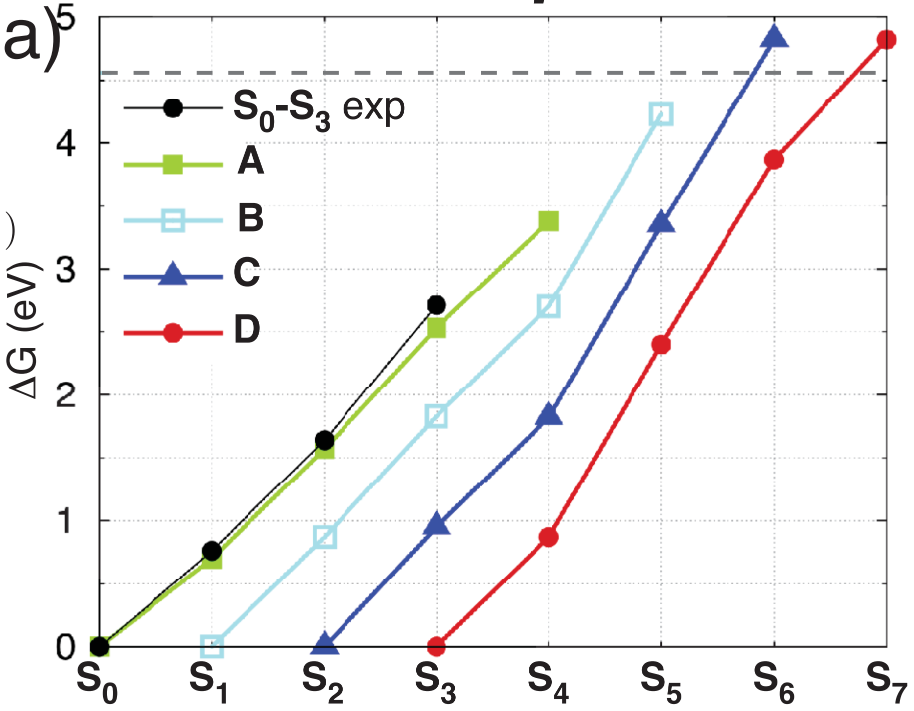
Study the evolution of the Ry4-POM complex along this cycle

Identify the intermediate capable to oxidize water

Identify the reaction mechanism for water oxidation and O2

Isolating the activated intermediate

Thermodynamics of electrochemical steps



- ✳Rossmeisl/Norskov approach

  Norskov et al., J. Phys. Chem. B 108, 17886 (2004)

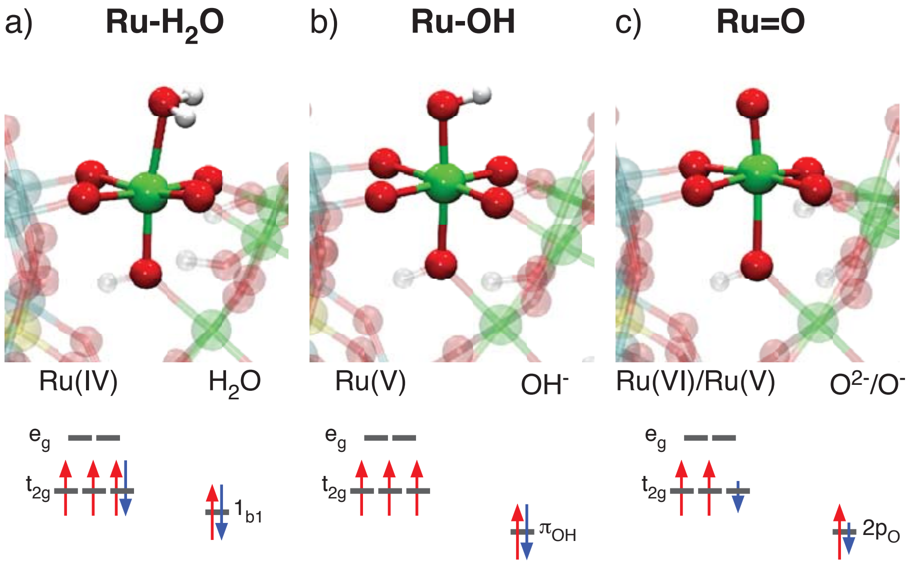
- ✳PCET - Set the reference potential to NHE

$$H^+ + e^- \leftrightarrow 1/2\,H_2 \qquad \mu(H^+) + \mu(e^-) = 1/2\mu(H_2)$$

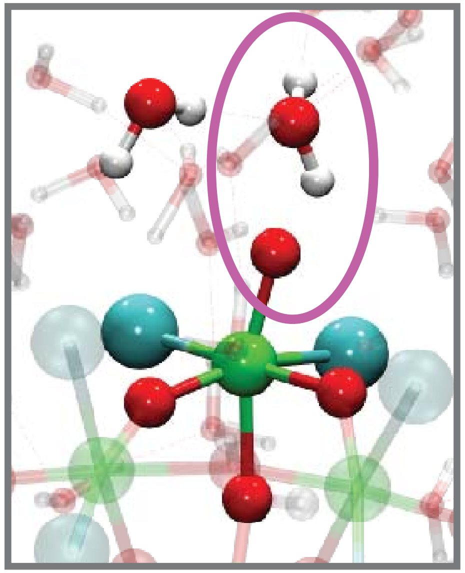
- ✳Compute DFT free energy difference

  (including ZPE and entropic terms)

$$\Delta G = \Delta E + \Delta ZPE + T\Delta S$$

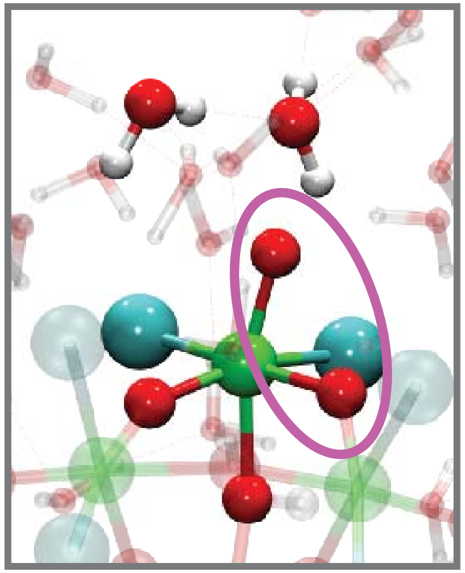


How is molecular O2 formed?



From the solvent?

- ✳nucleophilic attack of RuVI=O termination
- ✳The water that splits is from the solvent
- ✳Catalyst is not damaged and can be reactivated



From an O of the oxide core?

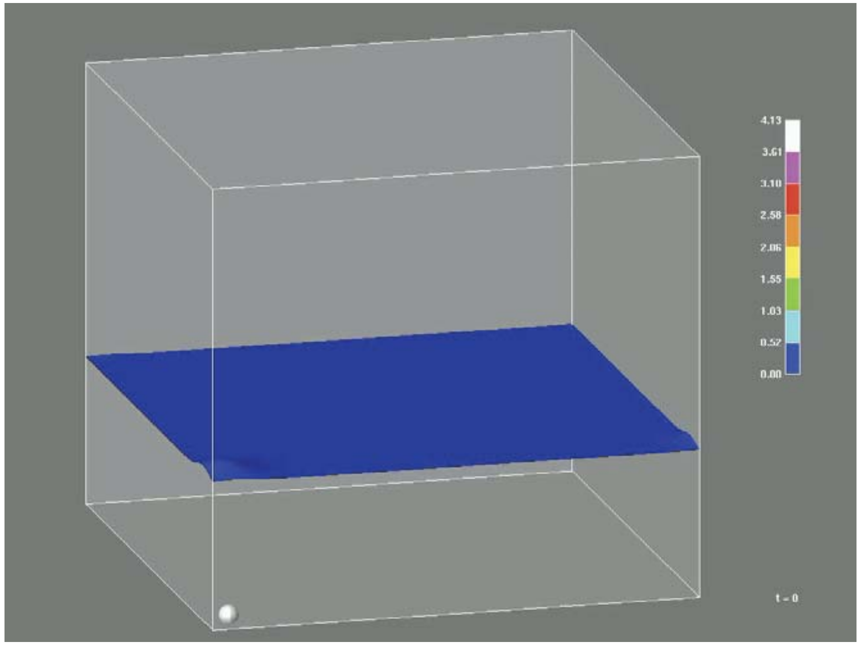
- ✳RuVI=O termination attacks the oxide cluster
- ✳Intermolecular mechanism without participation of water from the solvent
- ✳The water that splits is ligated
- ✳Catalyst is damaged and needs to be repared

Metadynamics

Simulating rare (activated) events without knowledge of the final state is even more challenging!

Reaction mechanism for water oxidation and O2 formation?

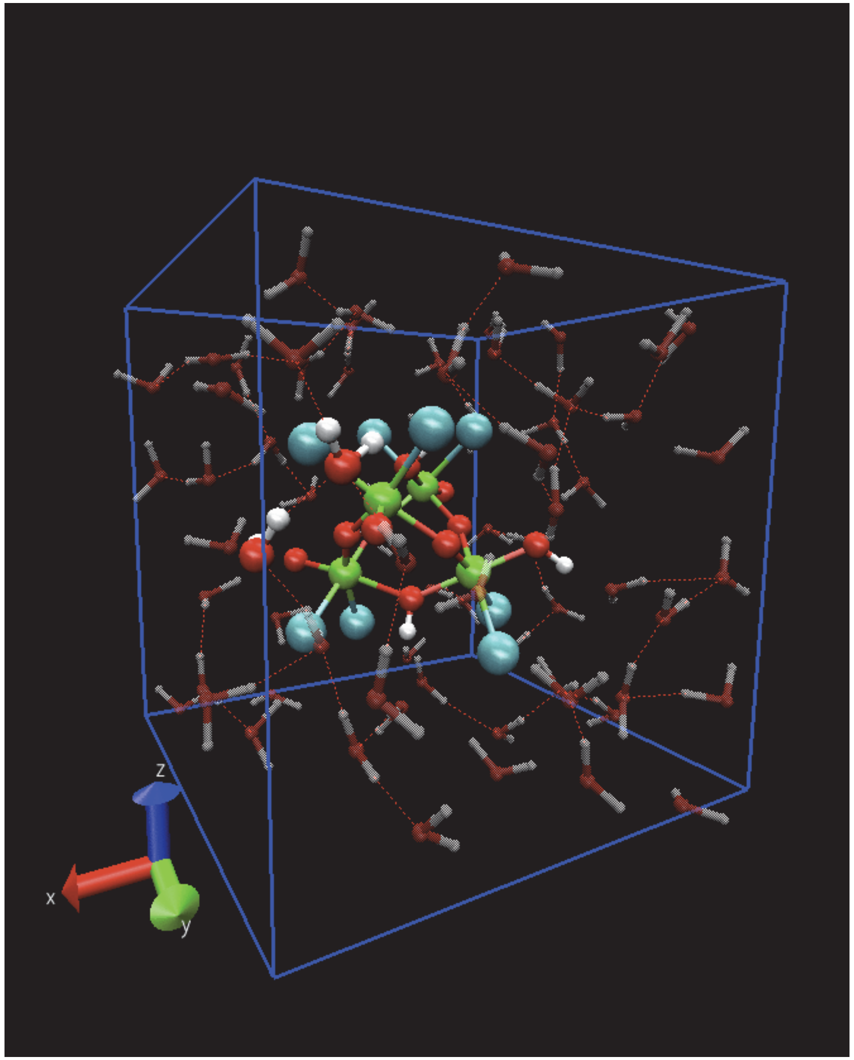
- Technique for accelerating rare events and reconstruct the free energy landscape
- Efficient exploration of configuration space
- Knowledge of final state is not required
- Biased and hystory-dependent MD



A. Laio and M. Parrinello, PNAS 99, 12562 (2002)

Metadynamics

Reaction mechanism for water oxidation and O2 formation?



S. Piccinin and S. Fabris, submitted

Metadynamics

Reaction mechanism for water oxidation and O2 formation?

✓ Provide insight into the working mechanisms of this catalyst

✓ Identify the intermediate capable to oxidize water: **$Ru^{V}=O\cdot$**

✓ Are 4 metal centers really necessary for an efficient catalyst? - NO!

✓ Address the free energy governing O2 formation

nucleophilic attack from the solvent

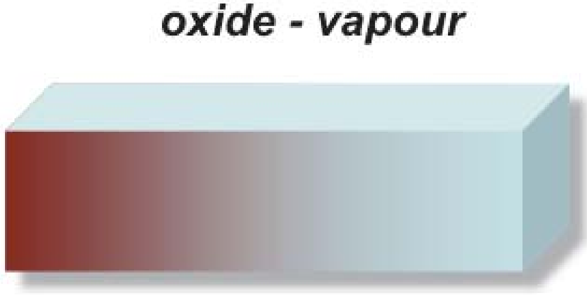
S. Piccinin and S. Fabris, submitted

Ab-initio thermodynamics

Dependency of the electrode/catalyst on T, p, V

The chemical environment influences the catalyst morphology, composition and reactivity

What is the most stable surface structure in the presence of a gas at given conditions of T and p?



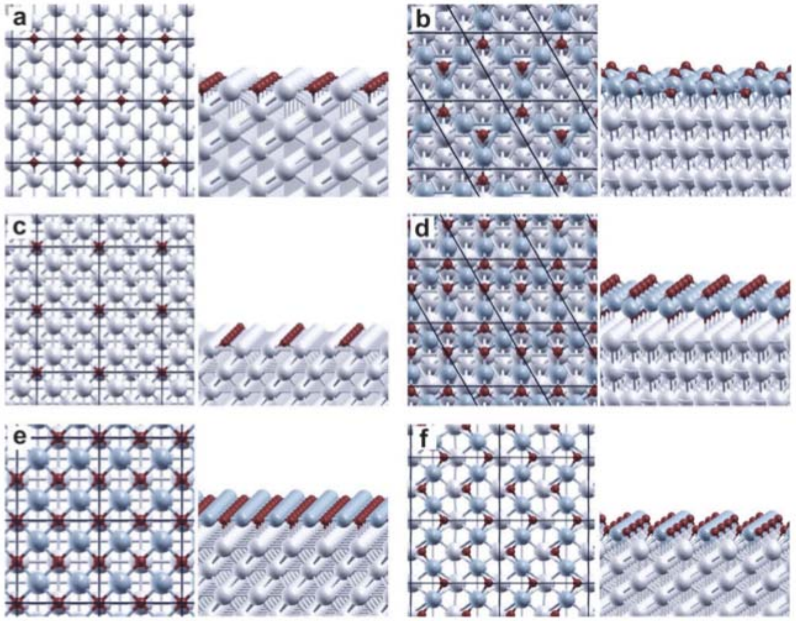
$$\mu_M = \mu_M^V$$

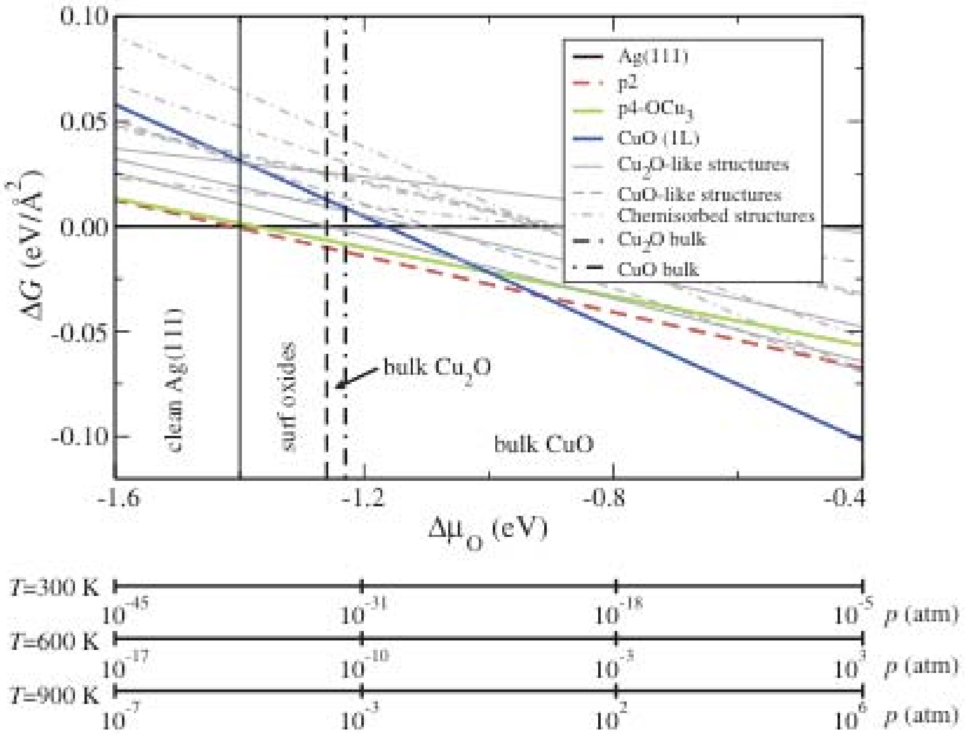
$$\mu_O = \mu_O^0 + \frac{1}{2} kT \ln p_{O_2}$$

$$\gamma(T,p) = \frac{1}{A} \left[G^S(T,p) - \frac{1}{m} N_M G_{MO}(T,p) \right]$$
$$- \Gamma_O \left(\frac{1}{n} G^0_{MO} - \frac{m}{n} \mu^0_M - \frac{1}{n} \Delta G^0 \right)$$
$$- \Gamma_O \frac{1}{2} kT \ln p_{O_2} \quad - N_A \, \mu_A(T, p_A)$$

Ab-initio thermodynamics

Prediction of exposed surface by Ag-Cu catalysts at given T and partial pressure of O2



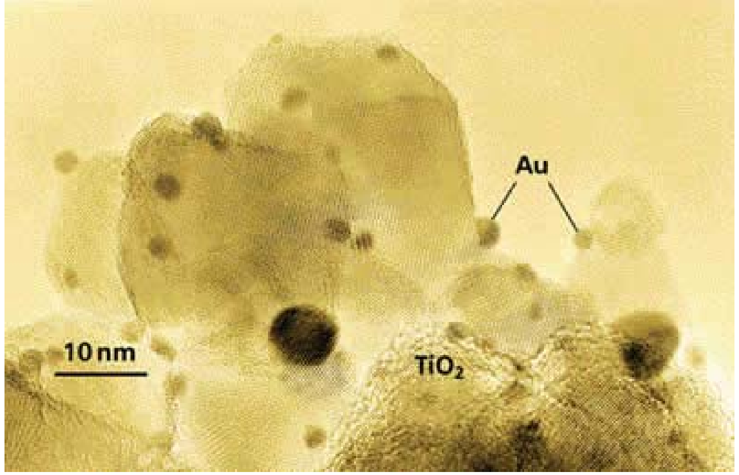


Piccinin et al., Surface Science 603 (2009) 1467–1475

Oxide supported metal catalysts

Metal nanoparticles supported by oxide substrates

- ENERGY: H_2 production, HC reforming, ...
- ENVIRONMENT: gas sensing, gas purification, ...
- DEVICES: fuel cells, photocatalysts, ...



Many fundamental issues of oxide surfaces are still unresolved

- Experimental difficulties: controlled synthesis, in-situ reactivity, ...
- Theory and simulation difficulties:
  - Alkaline earth oxides (MgO, ...)
  - Non reducible transition metal oxides (ZrO2, ...)
  - Reducible transition metal oxides (TiO2, ...)
  - Reducible rare-earth oxides (CeO2, ...)

Oxide supported metal catalysts

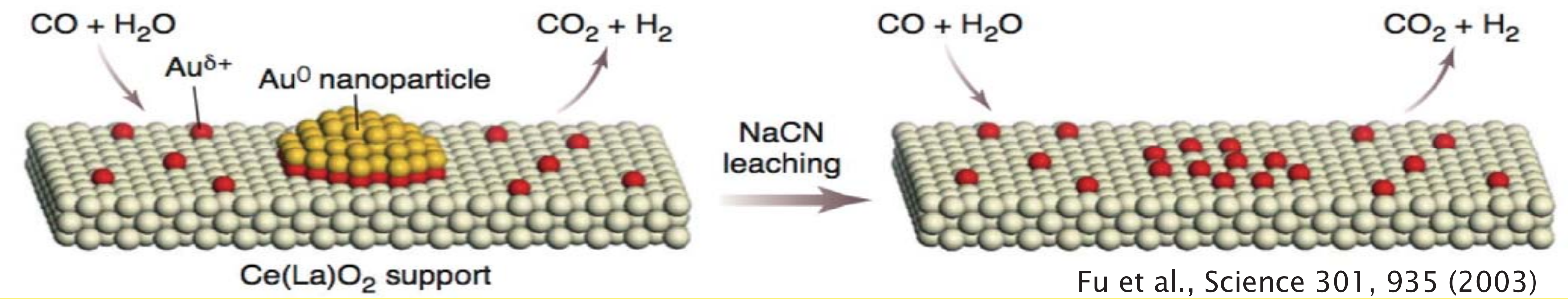
Metal nanoparticles supported by oxide substrates

Factors controlling reactivity:

- ➪ Type and size of metal nanoparticles
- ➪ Oxygen buffer capacity of oxide support

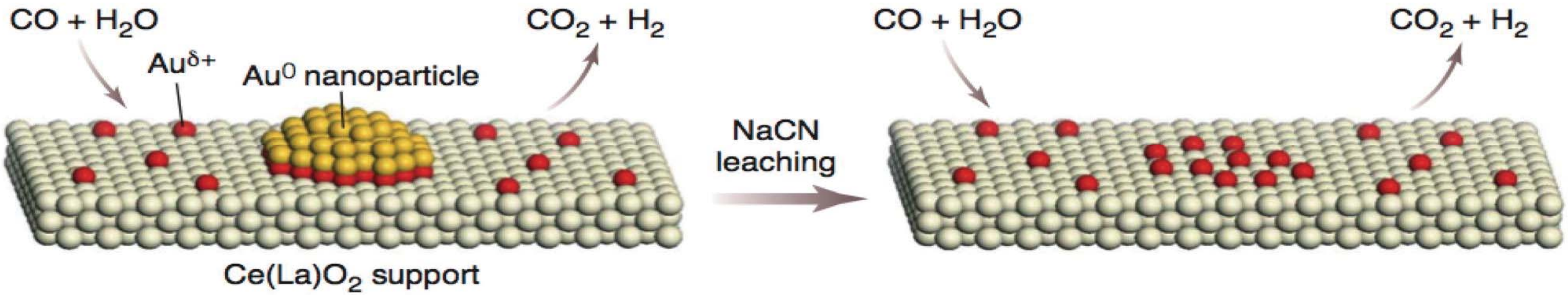
$$\mathrm{CeO_2} \rightleftarrows \mathrm{CeO_{(2-x)}} + \frac{x}{2}\mathrm{O_2}$$

- ➪ Oxidation state of supported metal



Fu et al., Science 301, 935 (2003)

Which are the active species on supported catalysts?



Water Gas Shift reaction

Fu et al., Science 2005: active species are isolated Au^{d+}

Rodriguez et al., xxx: no, they are neutral or negative Au species

CO oxidation

Guzman et al., JACS 2005: active species are isolated Au^{3+} or Au^{+}

Thermodynamics of Au adsorption

Free energy of adsorption of a Au adatom on the CeO2(111) surface

$$\boxed{\Delta G_a(T,p) = E_{slab}^{Au} - E_{stoi} + N_O^{vac}\mu_O(T,p) + N_{Ce}^{vac}\left[e_{CeO_2}^{bulk} - 2\mu_O(T,p)\right] - \mu_{Au}(T,p)}$$

Thermodynamics of Au adsorption

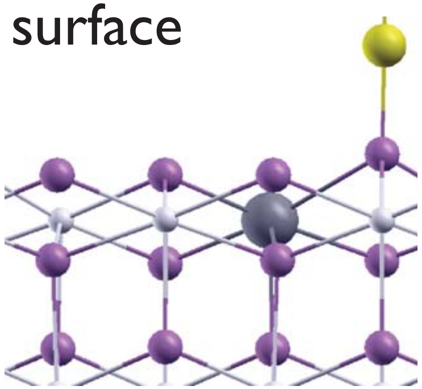
Free energy of adsorption of a Au adatom on the CeO2(111) surface

Only two relevant structures

Oxidative conditions

stoichiometric surface

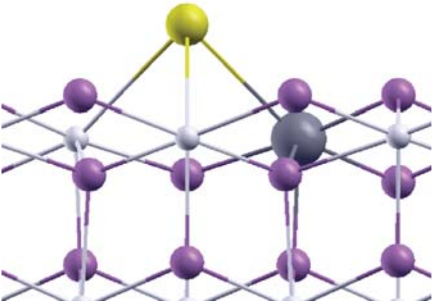
Au@CeO_2

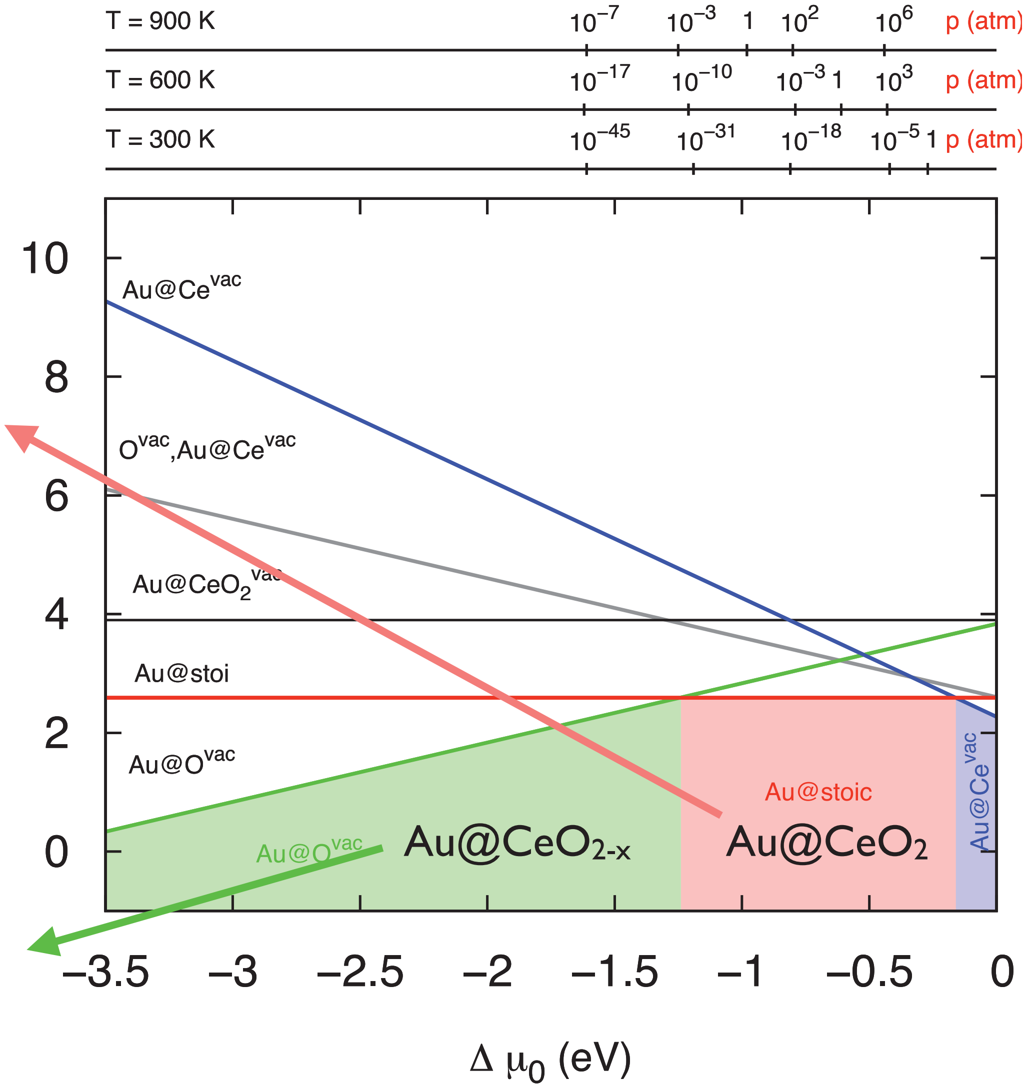


Reducing conditions

defective surface (O vacancy)

Au@CeO_{2-x}





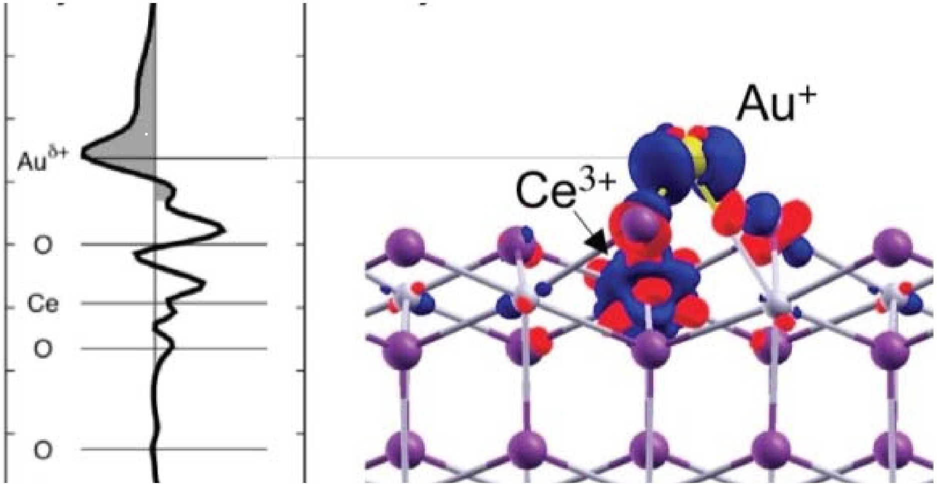
Supported Au ionic species

Charge transfer and electron localization effects at the metal/oxide interface

Au+ species in oxidizing conditions (CO ox)

~1 e

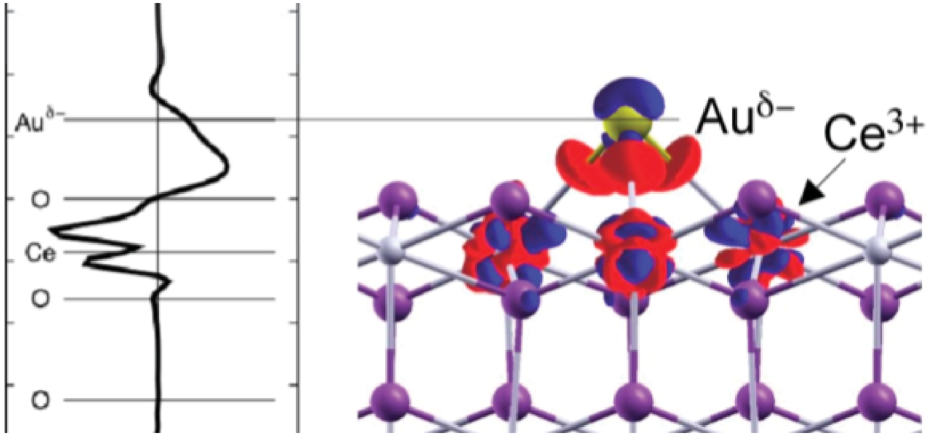
E(ads)
-1.18 eV



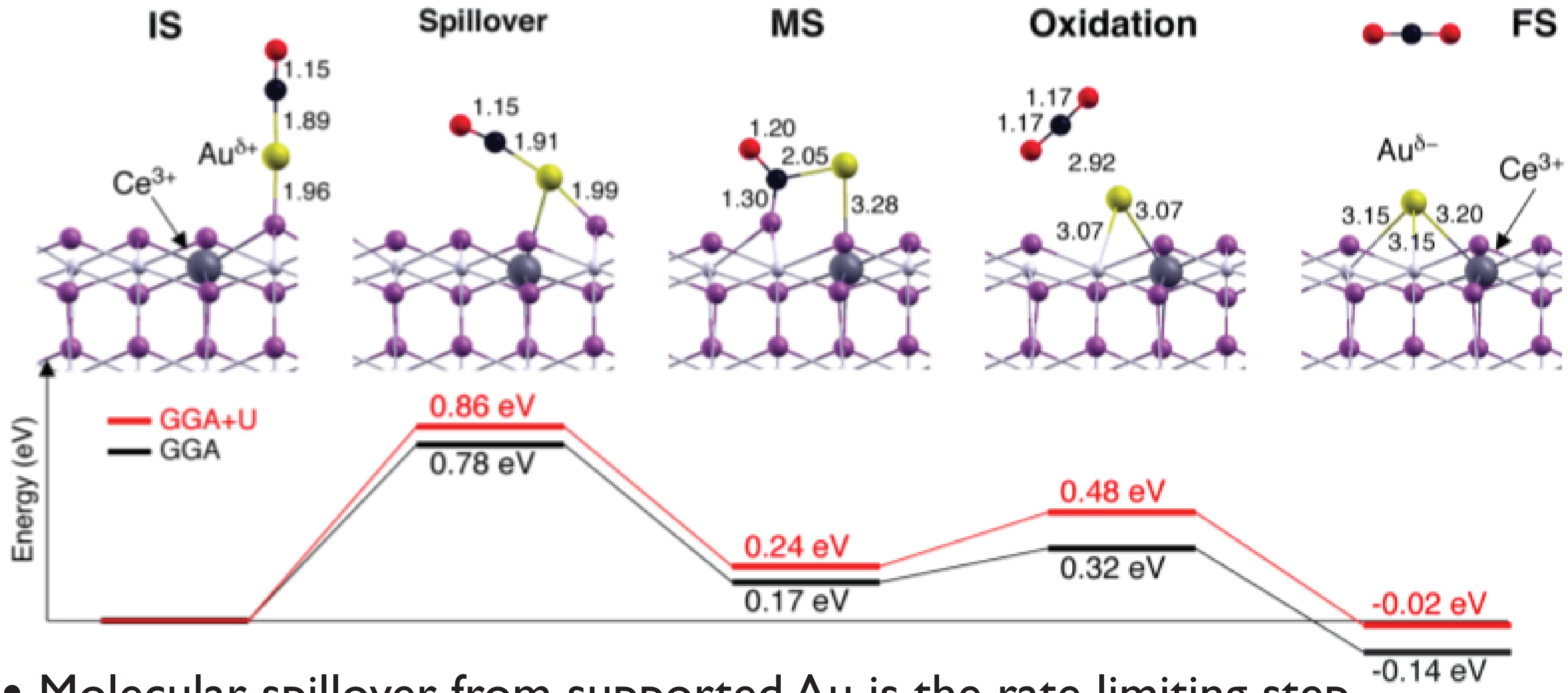
Au- species in reducing conditions (WGS)

~1 e

E(ads)
-2.29 eV



MEP for CO oxidation



- Molecular spillover from supported Au is the rate limiting step
- O vacancy formed during reaction attracts supported Au
- Charge reorganization and catalyst deactivation
- Results independent on the U parameter

Au+ species promotes CO oxidation but readily turns into inactive Au-

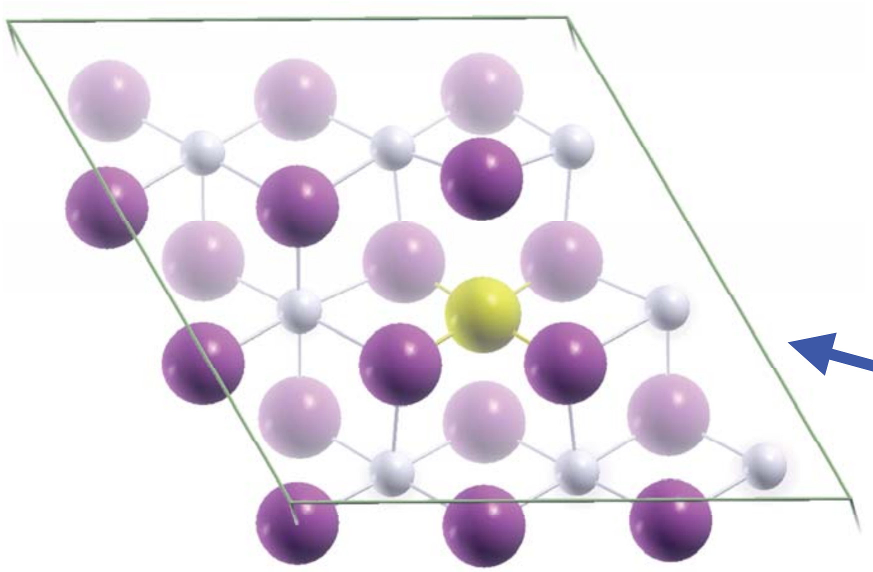
Thermodynamics of Au adsorption

Free energy of adsorption of a Au adatom on the CeO2(111) surface

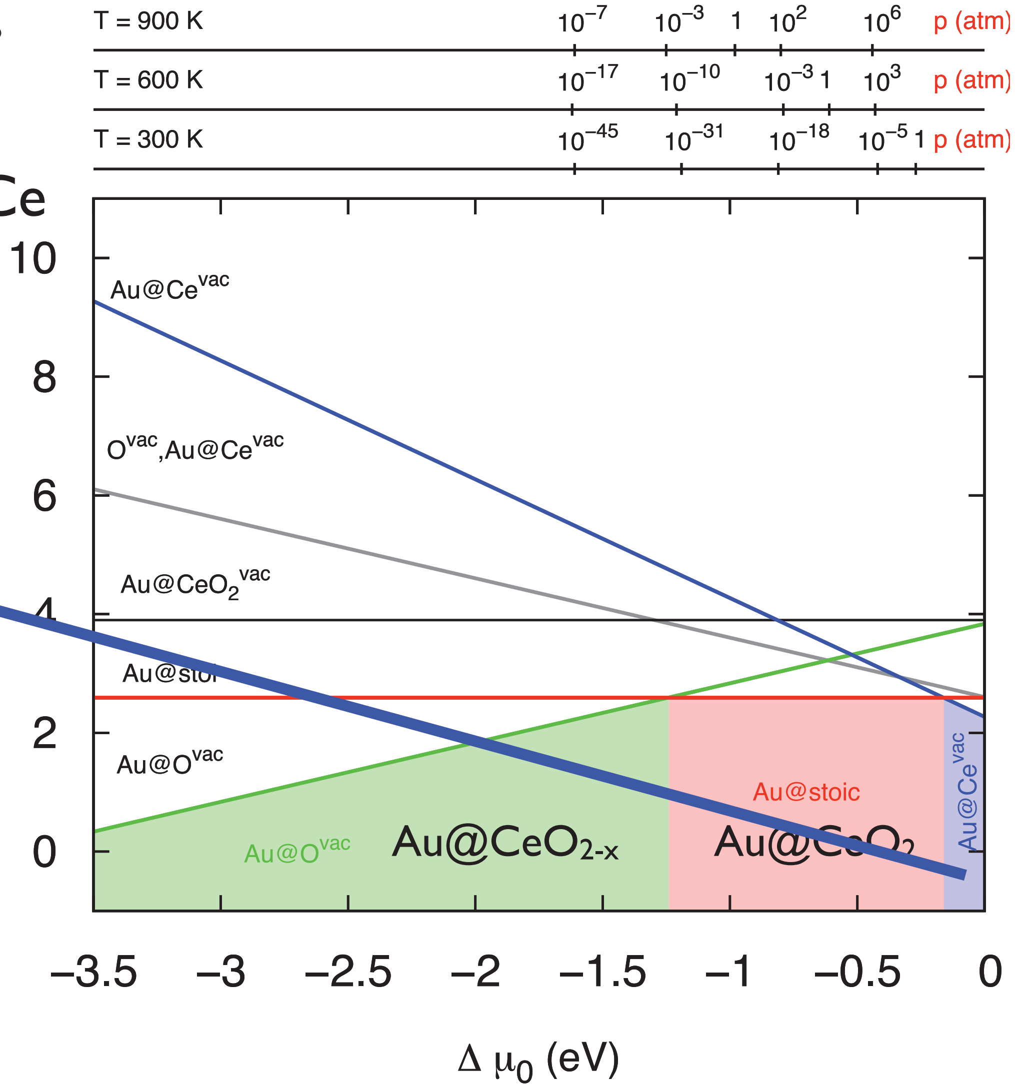
Only two relevant structures ...

Very oxidizing conditions:

solid solution: Au substitutional for Ce



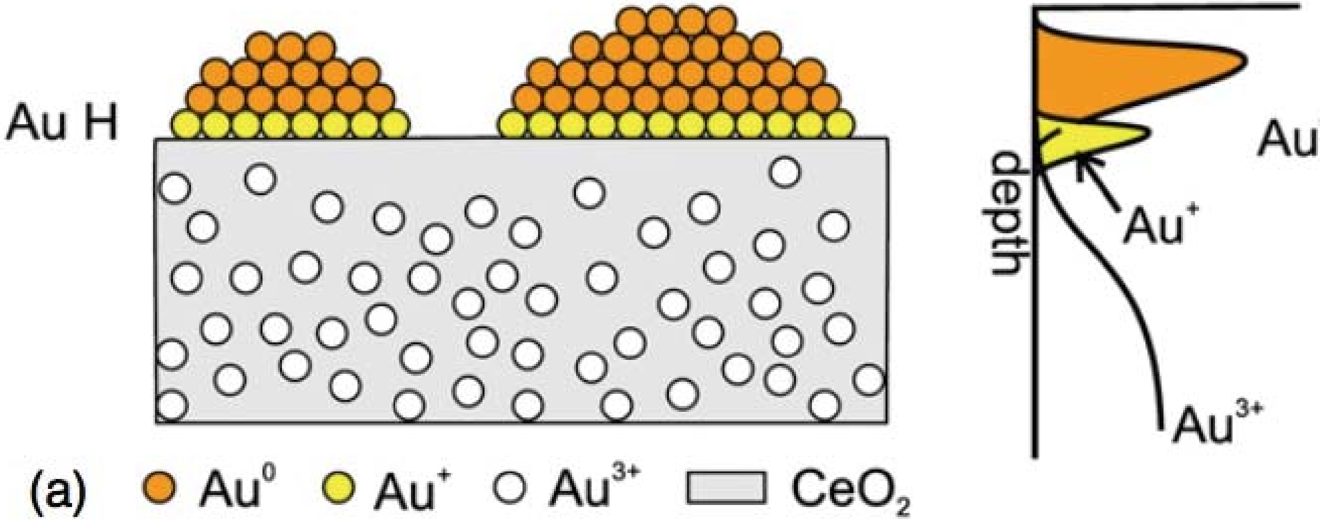
Squared-planar complex



(meta-)stability of solid-solutions

$Ce_{(1-x)}Au_xO_{(2-\delta)}$ solid solutions have been proposed on the basis of photoemission spectroscopy

J. Phys. Chem. 2005, 109, 2821; J. Chem. Phys. 2009, 130, 34703; J. Phys. D: Appl. Phys.. 2009, 42, 115301



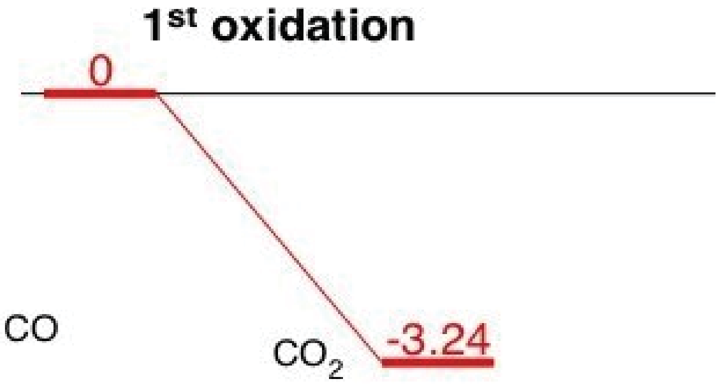
The stability of these systems is an issue of debate

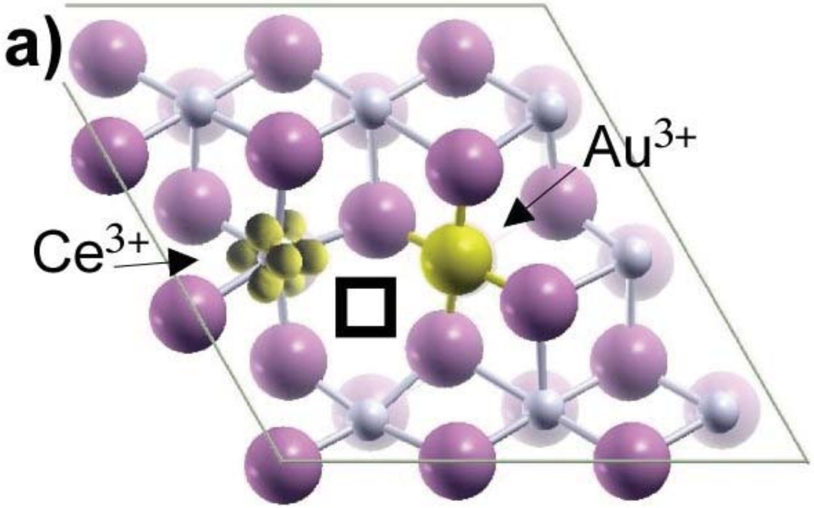
There is no direct crystallographic evidence for the existence and stability of these alloys

Measured solid solutions are kinetically but not thermodynamically stable?

Reactivity of AuO4 moiety in solid-solutions

AuO_4 moiety promotes direct oxidation of CO with no activation barrier





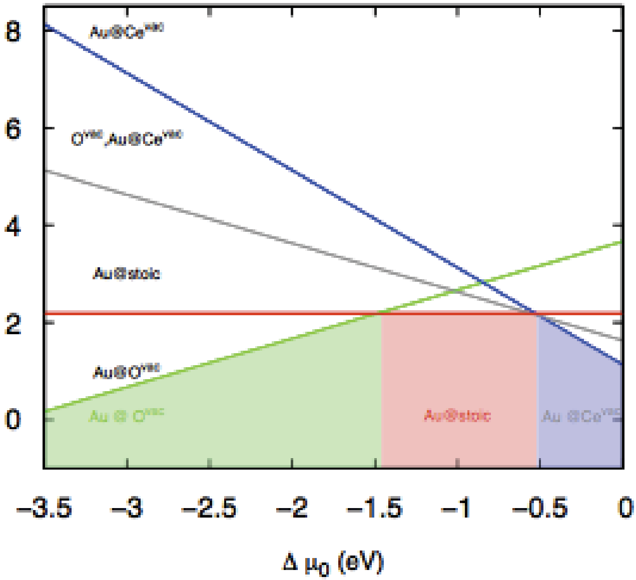
Materials screening: solid solutions

- Supported metal cations are most reactive species
- Most of the (expensive) metallic nanoparticle is wasted

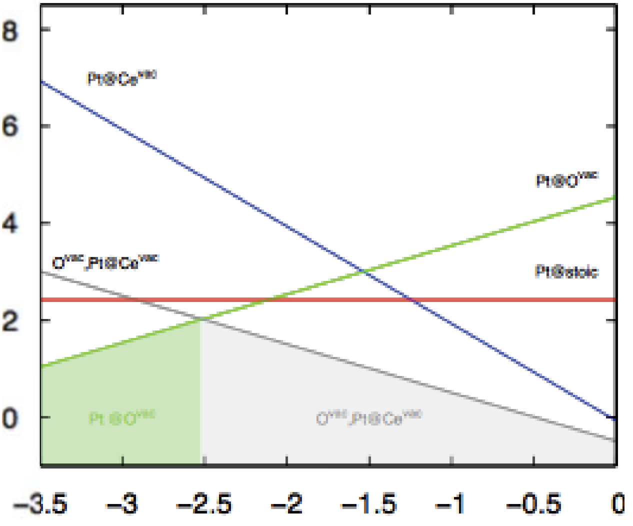
Is it possible to identify catalysts that maximize the exposed active cations and minimize the metallic particles?

$$\Delta G_a(T,p) = E_{slab}^{Au} - E_{slab}^{defec} - \mu_{Au}(T,p) + G_v(T,P)$$

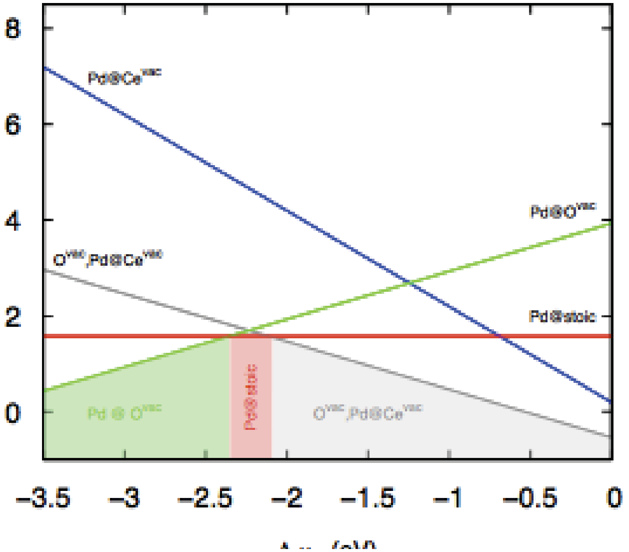
Au/CeOx



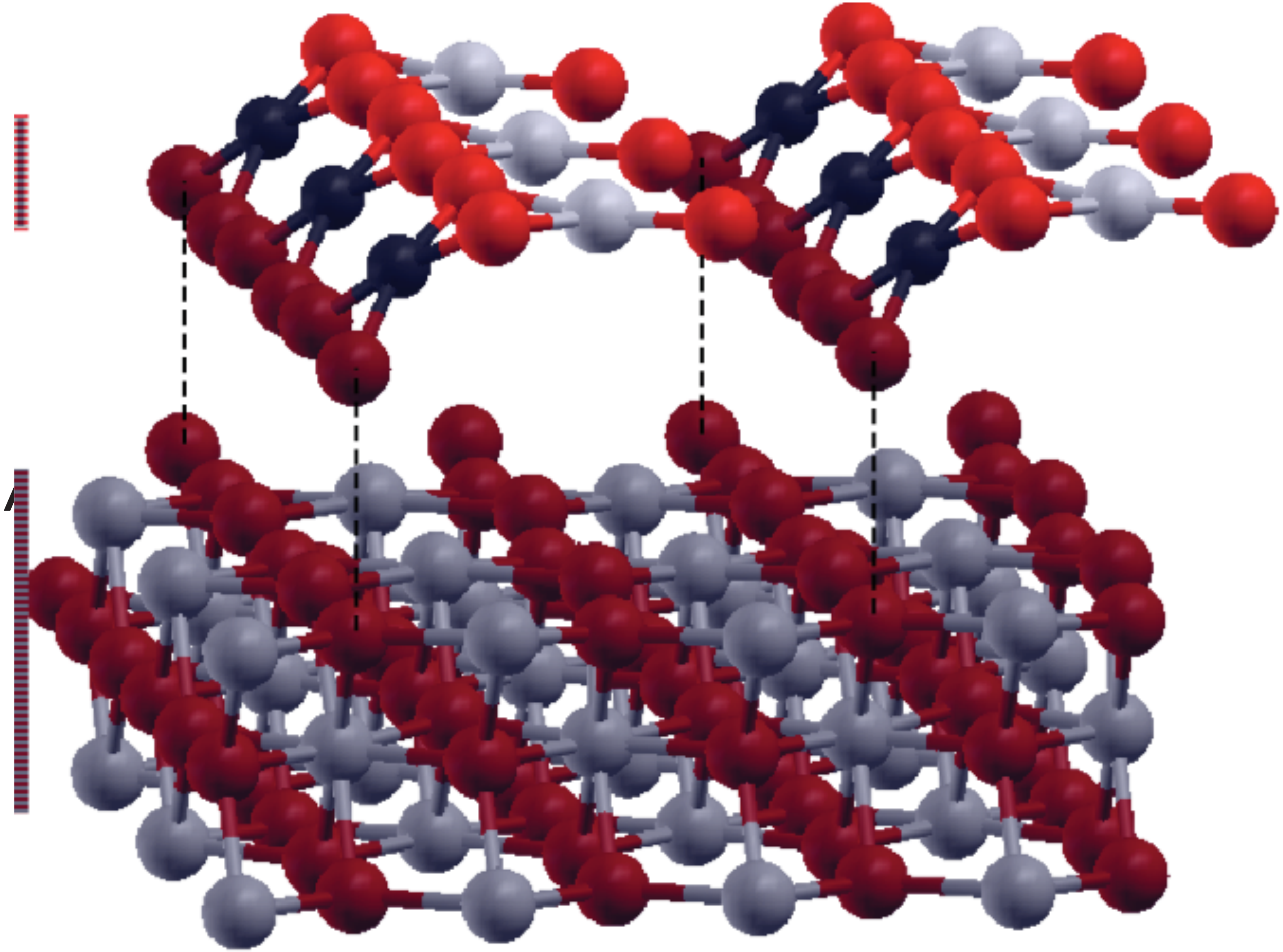
Pt/CeOx



Pd/CeOx



Materials screening: solid solutions



New catalysts:
a novel ordered PdCeO3 surface phase

Novel Pd/CeO2 catalysts show 5x increase in reactivity for methane activation

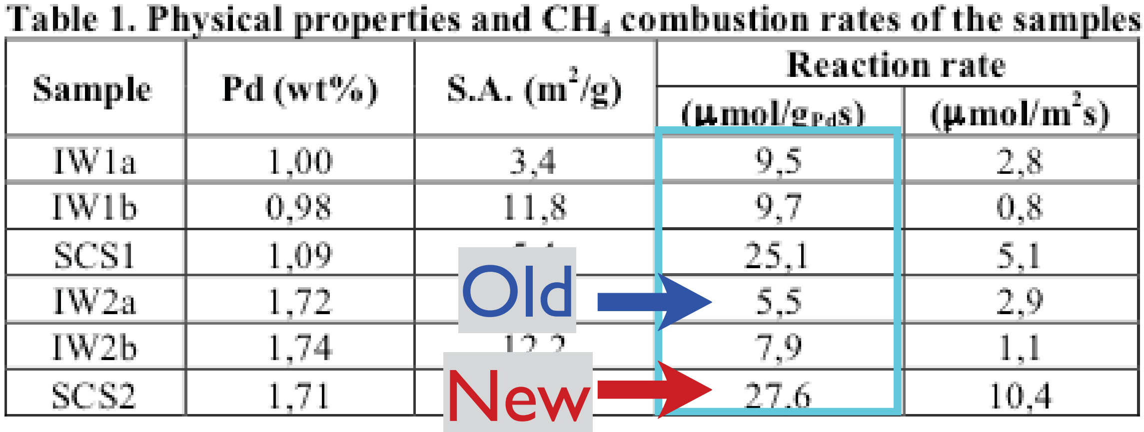
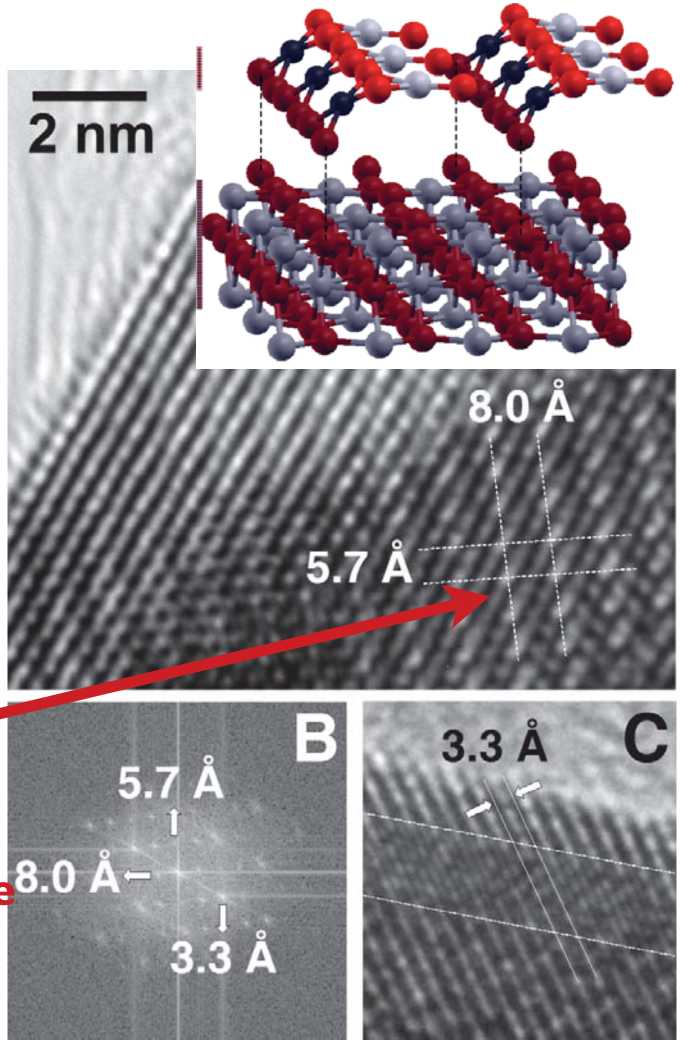


Table 1. Physical properties and CH_4 combustion rates of the samples

Sample	Pd (wt%)	S.A. (m^2/g)	Reaction rate ($\mu mol/g_{Pd}s$)	Reaction rate ($\mu mol/m^2s$)
IW1a	1,00	3,4	9,5	2,8
IW1b	0,98	11,8	9,7	0,8
SCS1	1,09	[illegible]	25,1	5,1
IW2a	1,72	[illegible]	5,5	2,9
IW2b	1,74	12,2	7,9	1,1
SCS2	1,71	[illegible]	27.6	10,4

A. Trovarelli, *University of UDINE*

HRTEM shows the presence of a new surface phase different than the standard (111) surface



J. Llorca, *University of Barcelona*

S. Colussi, MF, SF, et al., Angew. Chem. Int. Ed. 48, 8481 (2009)

WORKSHOP ON NEW MATERIALS FOR RENEWABLE ENERGY

17 - 21 October 2011

(ICTP, Miramare, Trieste, Italy)

The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, and the *International School for Advanced Studies* (SISSA), Trieste, are jointly organizing a ***Workshop on New Materials for Renewable Energy", to take place from 17 to 21 October 2011.***

This Workshop will address emergent materials and fundamental processes relevant in the context of renewable energy production, storage, conversion, and usage. The transition to sustainable energies from traditional energy sources based on fossil fuels or nuclear power is presently hampered by the low efficiencies or high costs of the available materials. The development of new materials by engineering their structure at the nano-scale is recognized to be the main bottleneck for both technology and basic science. Rational materials design holds the promise to drastically increase the performance of both renewable energy conversion and energy storage. In this sense, new materials are a key element for a possible transition towards a more sustainable energy economy.

The discovery and understanding of new physical and chemical processes underpins the development of a new generation of materials with improved performances, which could not be achieved by just incremental optimization of the existing materials. Understanding the interplay between structure, energetics and function of this new generation of materials makes this field also very appealing from a fundamental scientific point of view. Since the structure at the atomic scale is usually responsible for the observed efficiencies, this field is an ideal playground for collaborations between experiment and theory.

Another very important goal of this Workshop is to bring scientists from developing countries in contact with state of the art research and to enable them to carry out their own research in this domain. As most developing countries lie in areas with strong solar radiation, strong winds, or both, thanks to this large resource base, they are ideally suited for implementations of renewable energy technology. Also, the absence of a powerful energy infrastructure (grids) makes the use of small, decentralized, energy conversion devices very attractive.

TOPICS:

Topics covered in this workshop will include
- photovoltaics,
- artificial photosynthesis,
- fuel cells,
- electrocatalysis,
- batteries.

FORMAT:

The workshop will consist of invited lectures as well as contributed oral presentations. Also, a poster session will be organized. Participants willing to present a poster are invited to indicate this together with a title and a short abstract in the online application form.

PARTICIPATION

Scientists and students from all countries that are members of the United Nations, UNESCO or IAEA may attend the activity. As it will be conducted in English, participants must have an adequate working knowledge of this language. Although the main purpose of the Centre is to help researchers from developing countries through a programme of training activities within a framework of international cooperation, a limited number of students and post-doctoral scientists from developed countries are also welcome to attend.

As a rule, travel and subsistence expenses of the participants are borne by their home

ORGANIZERS:

Stefano FABRIS
(*CNR-IOM DEMOCRITOS and SISSA, Trieste, Italy)*

Ralph GEBAUER
(*ICTP, Trieste, Italy)*

INVITED SPEAKERS:

Vincenzo BALZANI*
    (Università di Bologna)
Marcella BONCHIO*
    (ITM-CNR and Università di Padova)
Christopher CRAMER
    (University of Minnesota)
Filippo DE ANGELIS
    (CNR and University of Perugia)
Sossina M. HAILE
    (California Institute of Technology)
Sharon HAMMES-SCHIFFER
    (Penn State University)
Nicola MARZARI
    (Oxford University)
Mohammad K. NAZEERUDDIN
    (Ecole Polytechnique Fédérale, Lausanne)
Simone PICCININ
    (CNR-IOM DEMOCRITOS, Trieste)
Xavier Sala ROMAN
    (Universitat Autònoma de Barcelona)
Serdar SARICIFTCI
    (University of Linz)
Robert SCHLÖGL
    (Fritz Haber Insitute, Berlin)
Michiel SPRIK
    (Cambridge University)
Carlo TALIANI
    (CNR Bologna)
Omar M. YAGHI
    (University of California, Los Angeles)
Teketel YOHANNES
    (Addis Ababa University

Computational modeling of catalytic materials for H_2-based technologies

THANK YOU!

Simone Piccinin

Matteo Farnesi

Changru Ma

Stefano Fabris

fabris@sissa.it

CNR-IOM DEMOCRITOS Simulation Center

SISSA - Scuola Internazionale Superiore di Studi Avanzati

Trieste - ITALY

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