

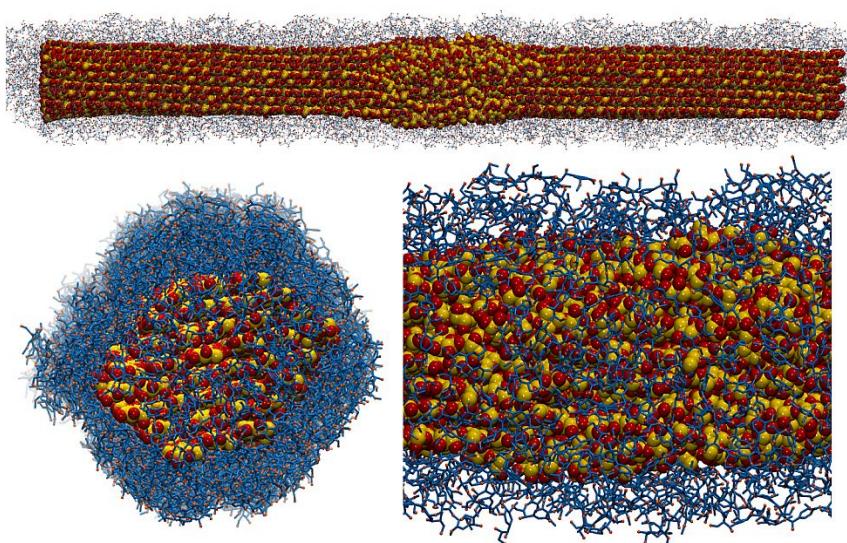
Introduction to first-principles modeling of catalysis at surfaces

Bryan R. Goldsmith

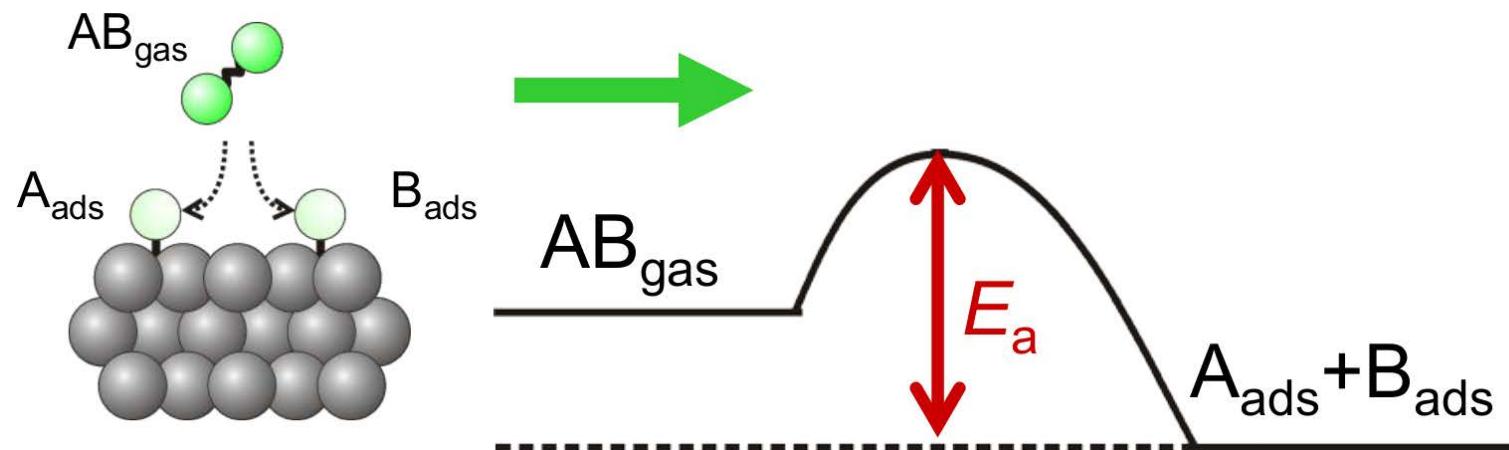
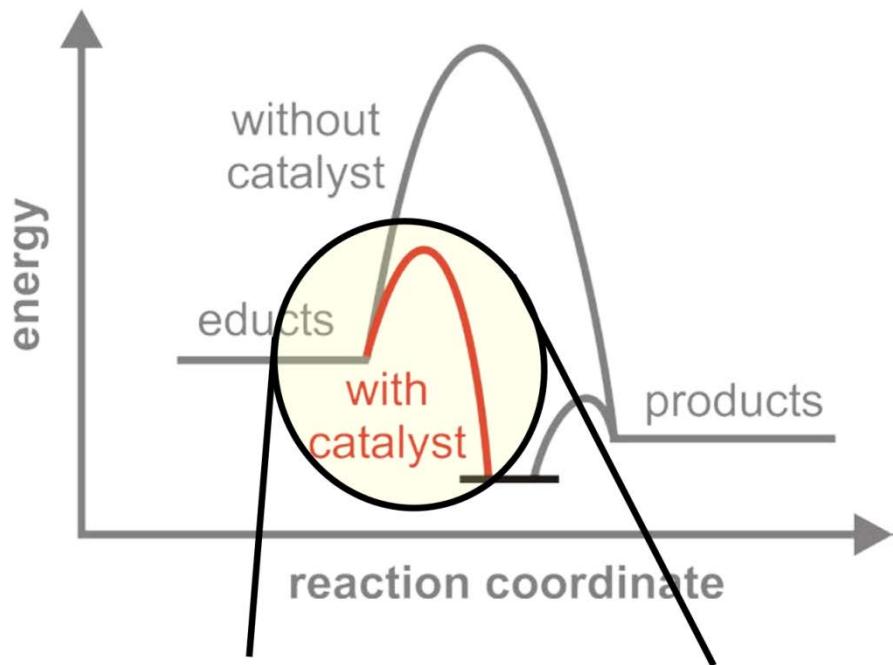
Fritz-Haber-Institut der Max-Planck-Gesellschaft
Theory Department



Catalysis is a multibillion-dollar industry
and has a profound influence in everyday life



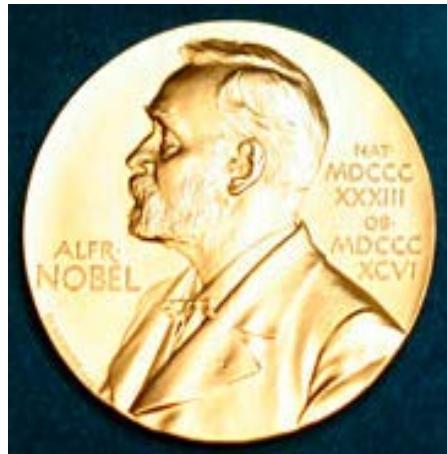
Catalysts lower the activation barrier of a reaction without being consumed



Early Nobel prizes for catalysis



Wilhelm Ostwald
"investigations into the fundamental principles governing chemical equilibria and rates of reaction", 1909



"for discoveries that confer the greatest benefit on mankind"



Paul Sabatier
"for his method of hydrogenating organic compounds in the presence of finely disintegrated metals", 1912



Fritz Haber, Berlin-Dahlem
"for the synthesis of ammonia from its elements", 1918



Irving Langmuir
"for his discoveries and investigations in surface chemistry", 1932



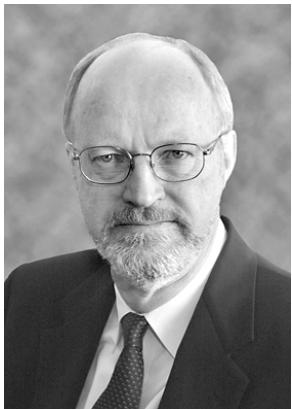
Cyril Hinshelwood
"for researches into the mechanism of chemical reactions", 1956

Some 21st-century Nobel prizes for catalysis

What contributions can *ab initio* modeling provide to the catalysis field?



Yves Chauvin, Lyon, France, 2005



Robert Grubbs,
Pasadena, CA, 2005

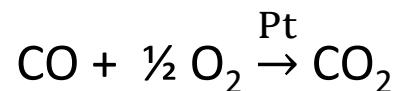


Richard Schrock
Boston, MA, 2005

"for the development of the
metathesis method in organic synthesis"



Gerhard Ertl
Fritz-Haber-Institut, Berlin
"for his studies of chemical processes on solid surfaces", 2007

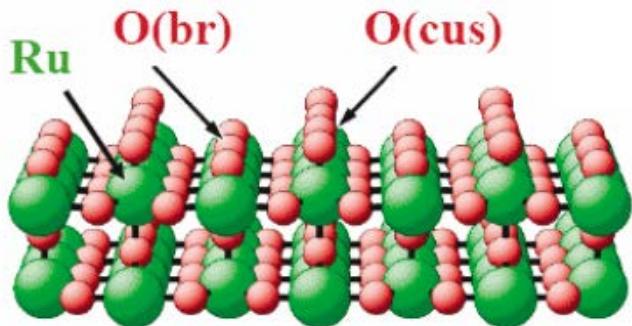


Outline of this block course

- 1) Introduction to computational catalysis and first-principles modeling
- 2) Cluster models, slab models, *ab initio* thermodynamics and its applications
- 3) Transition state theory and potential energy surfaces
- 10 minute break
- 4) Computational screening of catalysts and the use of ‘descriptors’
- 5) Topical Examples
 - Disintegration and redispersion of noble metal nanoparticles
 - Modeling isolated catalyst sites on amorphous supports

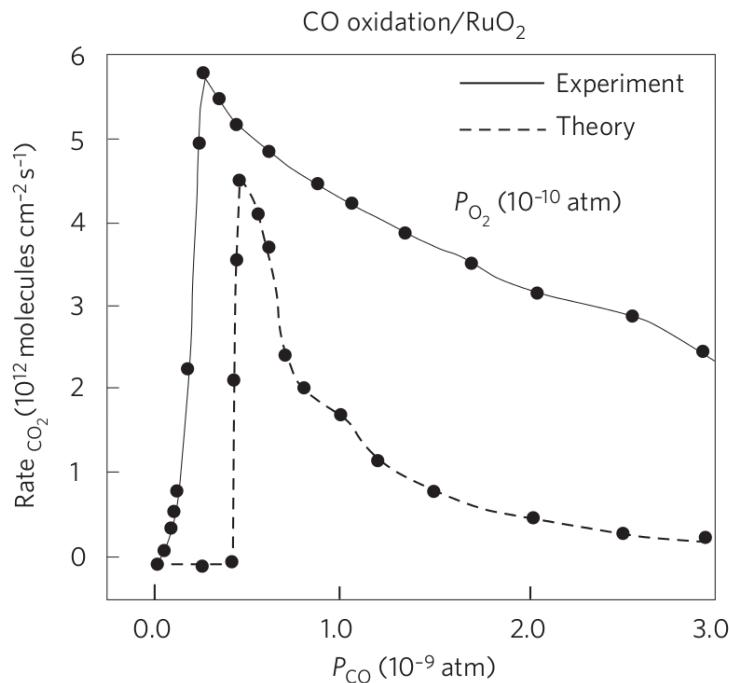
Computational modeling can assist in understanding catalysis

CO oxidation at RuO₂

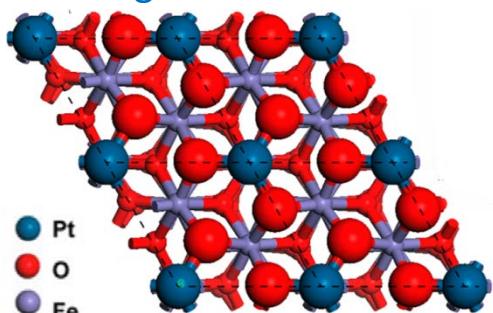


[1] K. Reuter, et al.
Phys. Rev. Lett. 93, 116105 (2004)

**Many opportunities
for improving catalysts remain**

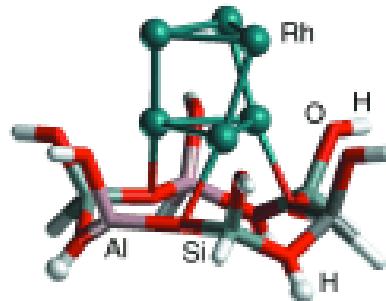


Single atoms



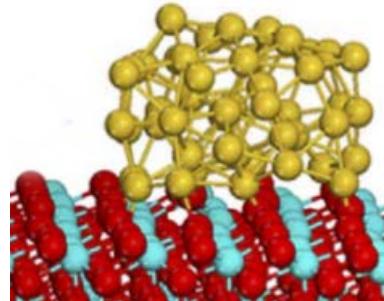
Single Pt atoms
dispersed on FeO_x

Nanoclusters



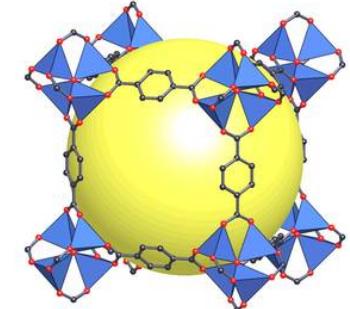
Rh₆ nanocluster
supported by a zeolite

Nanoparticles



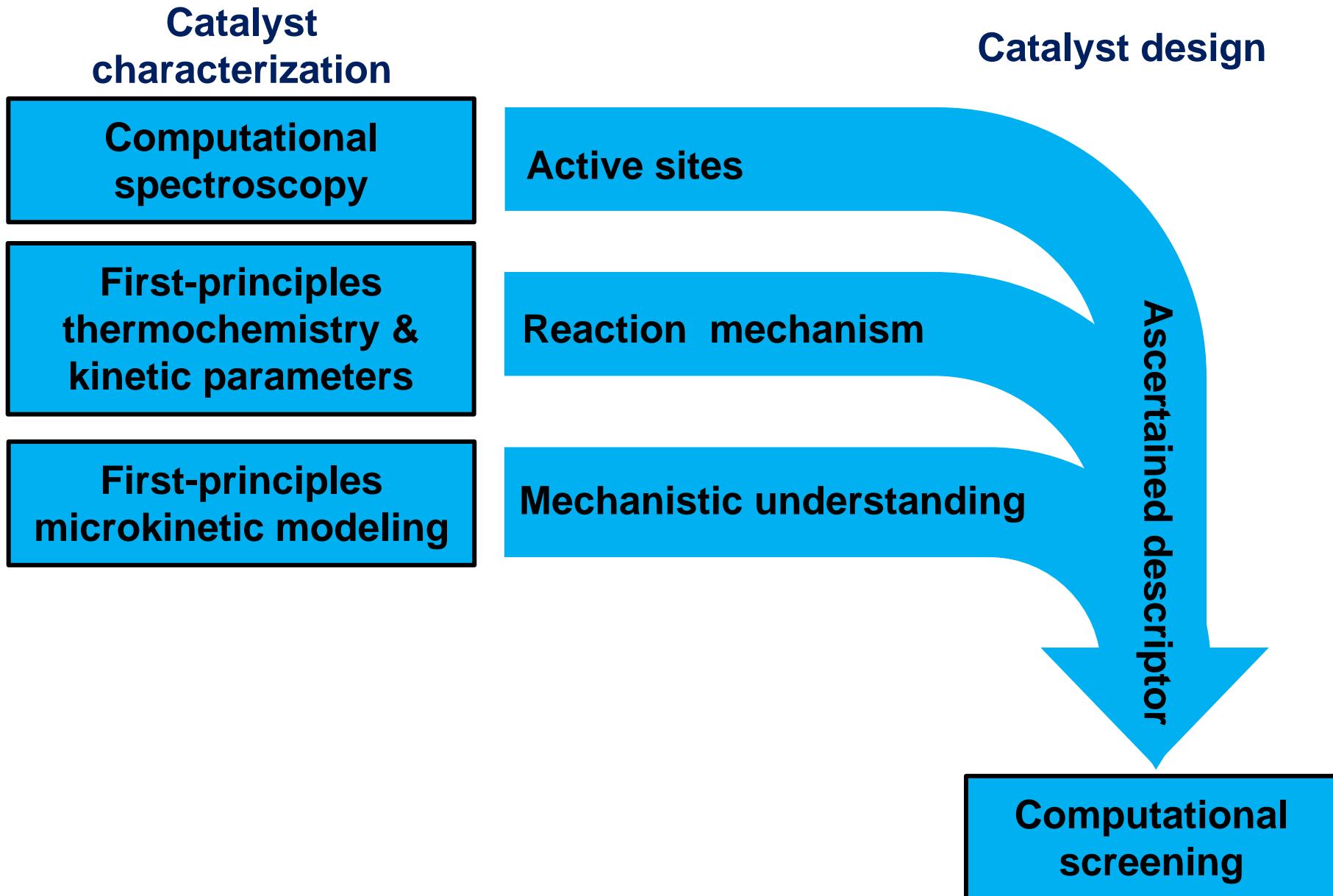
Gold nanoparticle
supported by CeO₂

Metal-organic frameworks

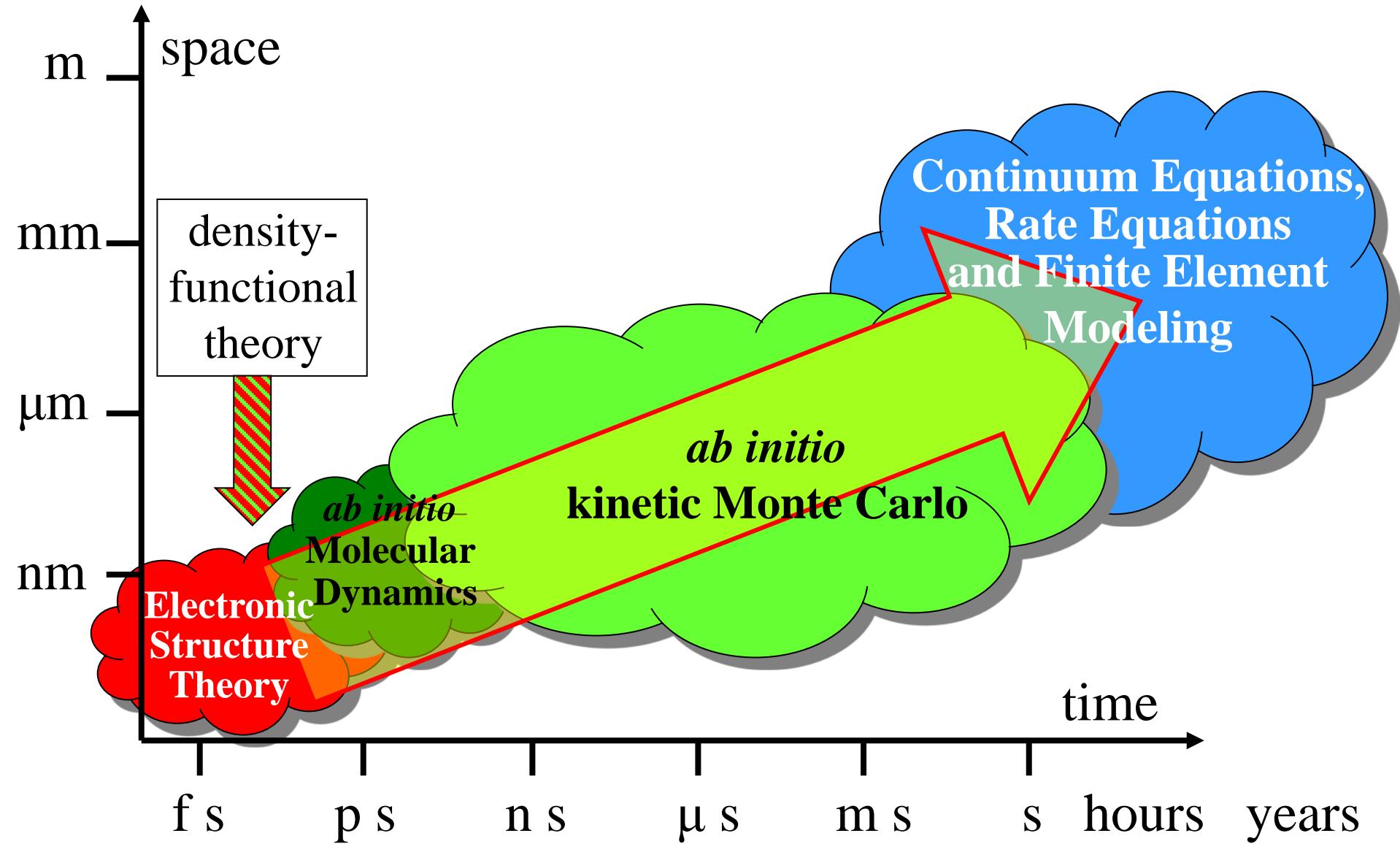


The MOF-5
lattice structure

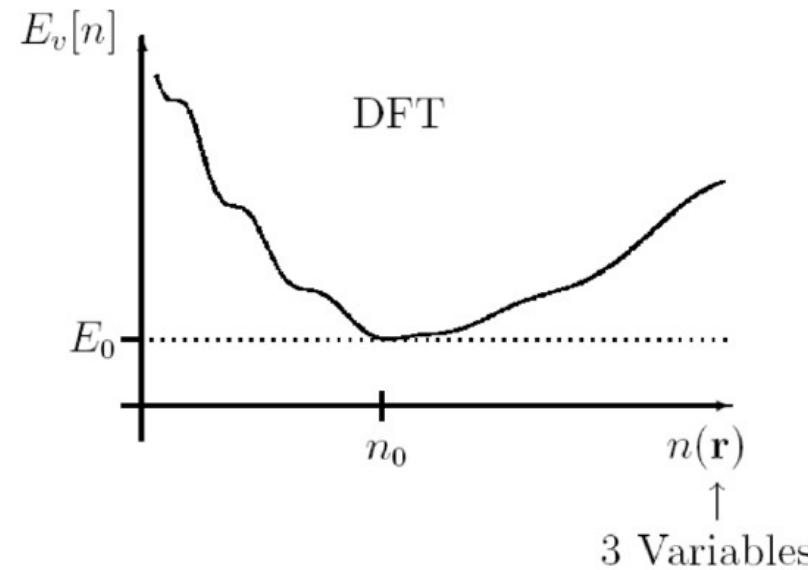
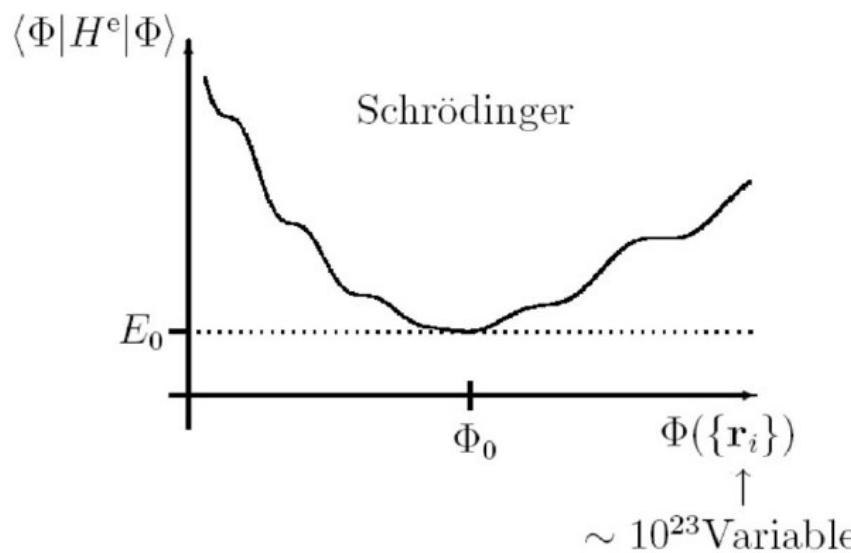
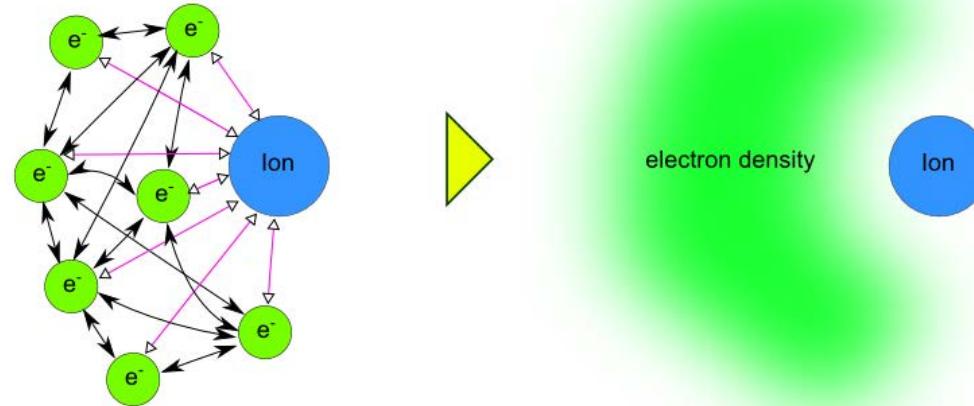
The dream: computational catalyst design



Toward realistic time scales via simulation



The electron density contains all the information and is more tractable than the wave function



Electronic structure theory approaches

Potential energy for fixed nuclear positions $\{\mathbf{R}_I\}$:

$$E_0(\{\mathbf{R}_I\}) = \text{Min}_{\Psi} \langle \Psi | H^e\{\mathbf{R}_I\} | \Psi \rangle$$

Wavefunction based methods (Quantum Chemistry)

Hartree-Fock, post Hartree-Fock (MP2, coupled cluster,...)

Density-functional theory

$\Psi = \Psi[n(\mathbf{r})]$ (Hohenberg-Kohn, 1964)

$$E_0(\{\mathbf{R}_I\}) = \text{Min}_{n(\mathbf{r})} E_{\{\mathbf{R}_I\}}[n]$$

$$E_{\{\mathbf{R}_I\}}[n] = T_s[n] + \int d^3r v_{\{\mathbf{R}_I\}}^{\text{nuc}}(\mathbf{r})n(\mathbf{r})$$

$$+ \frac{1}{2} \int \int d^3r d^3r' \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + E^{\text{xc}}[n]$$

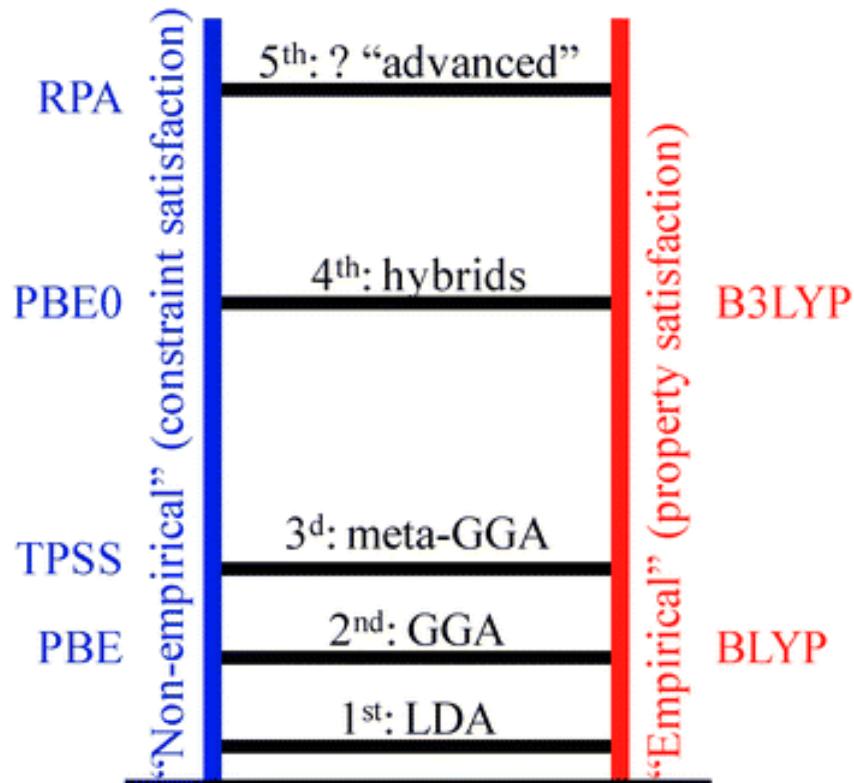
(Kohn-Sham, 1965)

$$E_{LDA}^{\text{xc}}[n] = \int d^3r n(r) \varepsilon^{\text{xc}}(n_o) \Big|_{n_o=n(r)}$$

$$E_{GGA}^{\text{xc}}[n] = \int d^3r n(r) \varepsilon^{\text{xc}}(n_o, \nabla n_o) \Big|_{n_o=n(r)}$$

Density functional theory (DFT) is widely applied to model catalysis at surfaces

the choice of the exchange-correlation (XC) functional
is critical for accurate predictions!



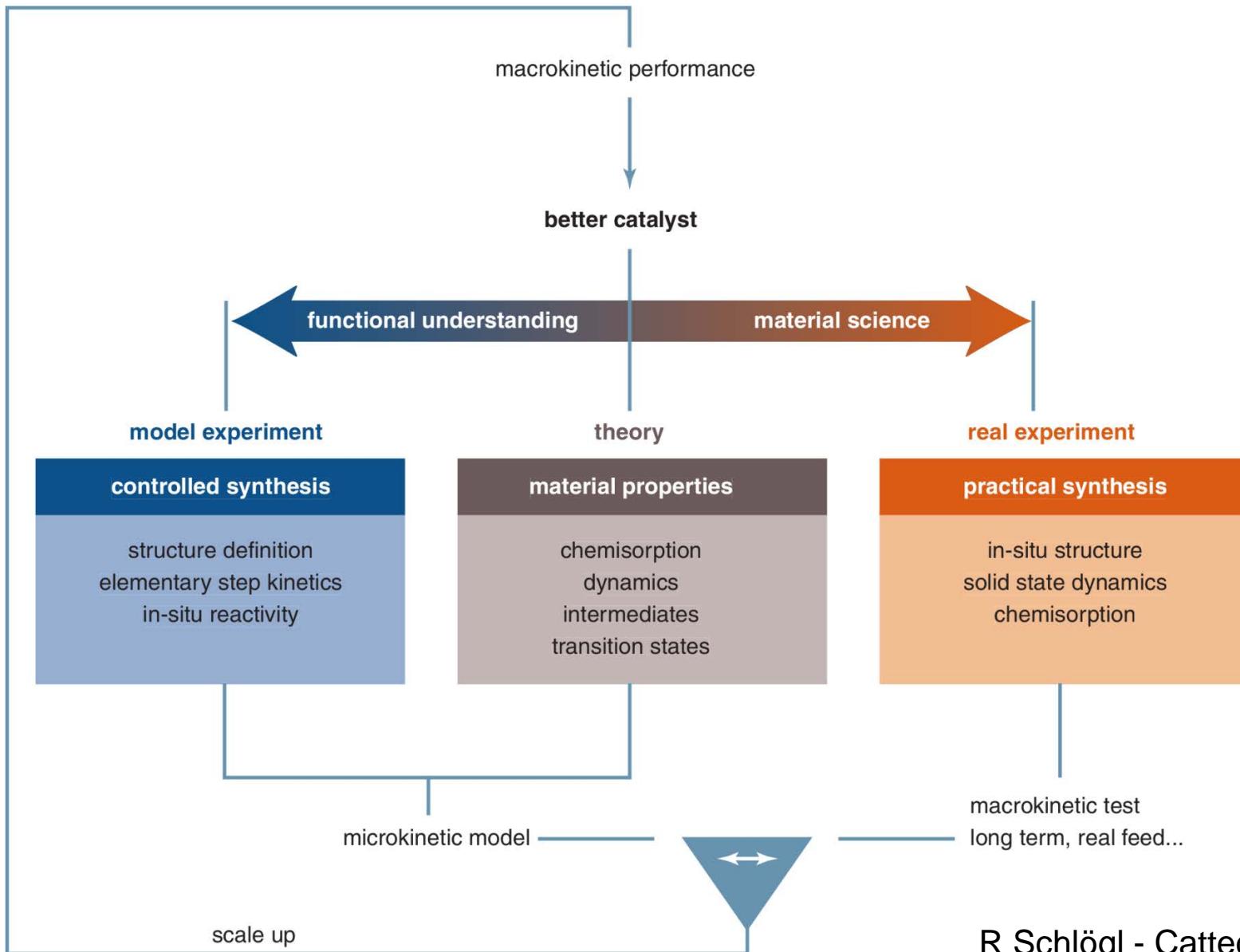
Practitioner level
GGA (metals)
Hybrids (molecules, insulators)

Major problems
Self-interaction error
Van der Waals interaction

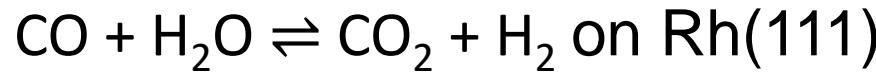
Inaccuracies in binding energies and
activation barriers of order 0.2 – 0.4 eV!

J. P. Perdew and K. Schmidt,
AIP Conf. Proc., 577, 1 (2001)

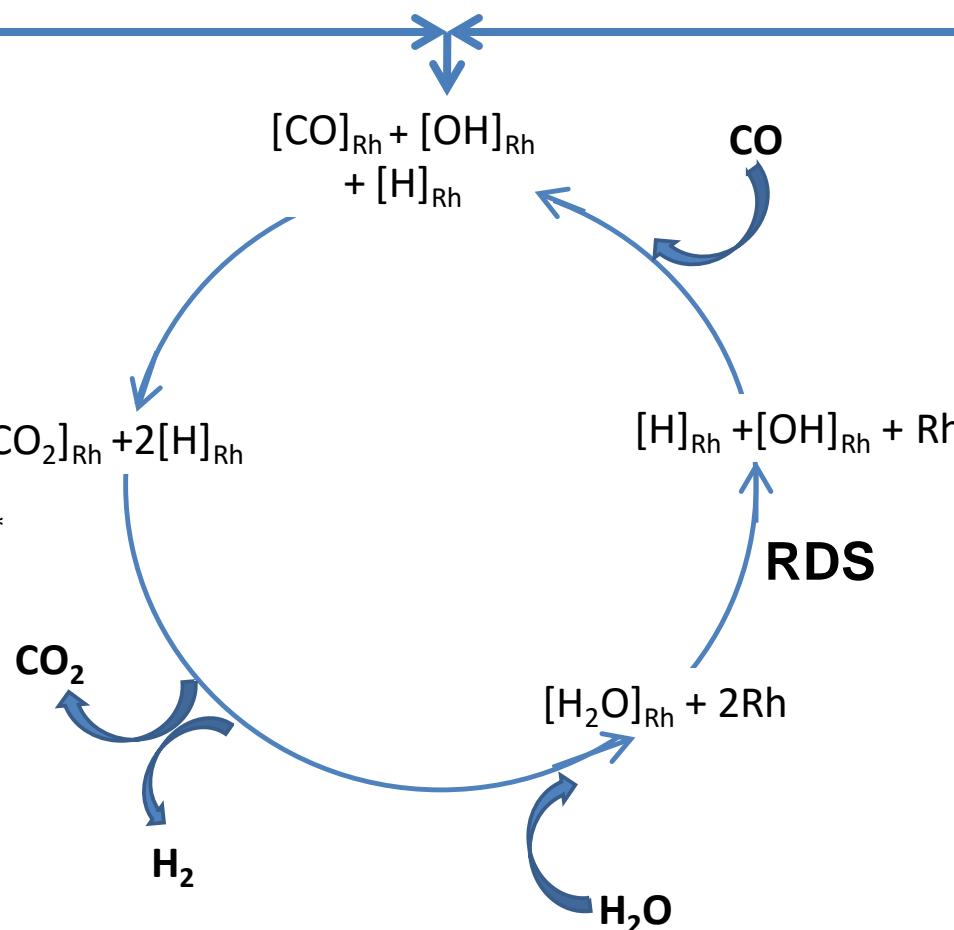
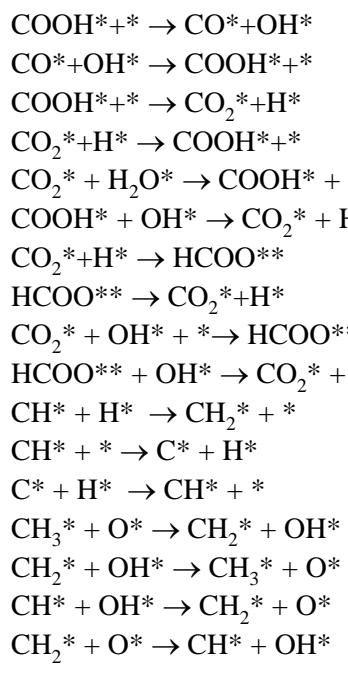
Theorists and experimentalists should work closely together from *the beginning* of a project. Theory can facilitate the development of catalysts and the understanding of reactions.



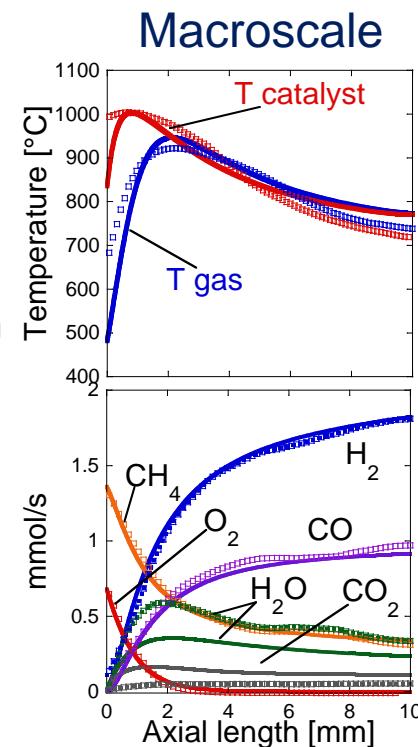
Understanding the full catalytic cycle for even ‘simple’ surface reactions is challenging



Microscale



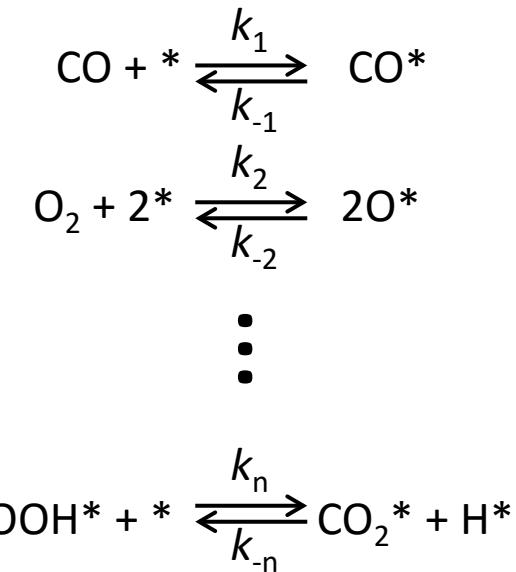
~ 10² potential steps
@ different coverages



Phenomenological models

Determine rate constants
by fitting to experimental kinetic data

A multiparameter fit problem



Challenges

Measure rates most sensitive to rate-determining steps (RDS)

Perform experiments under wide range of operation conditions

Different rate-determining step?

Different surface structure and composition?

Insufficient data (in particular on intermediates) to fully determine mechanism

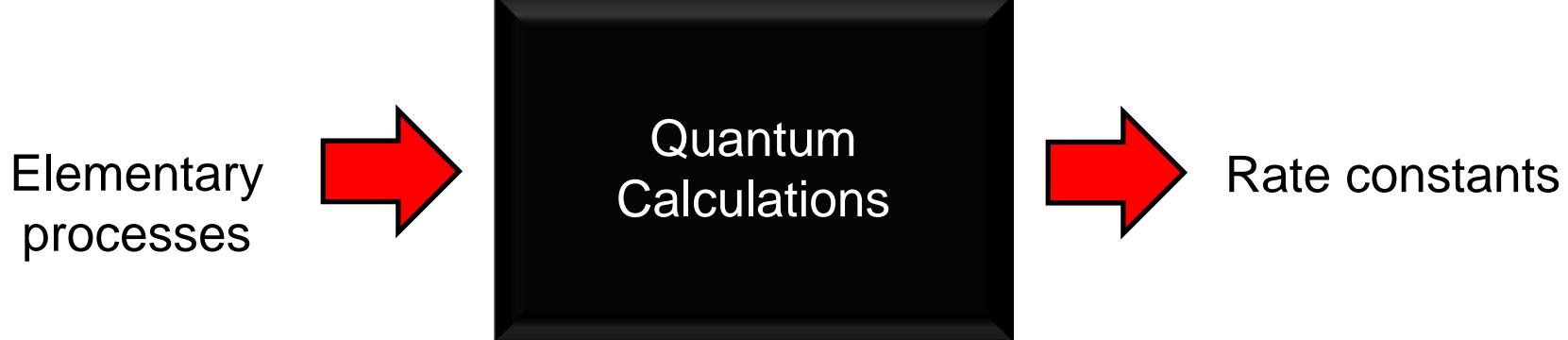
Branched/multi-step mechanisms

From phenomenological models to *ab initio*

Different reaction mechanisms can fit existing data equally well
(more the norm than exception)

- Nullifies the objective of microkinetic modeling to generate mechanistic understanding
- Derived rate constants then have no microscopic meaning (effective parameters)

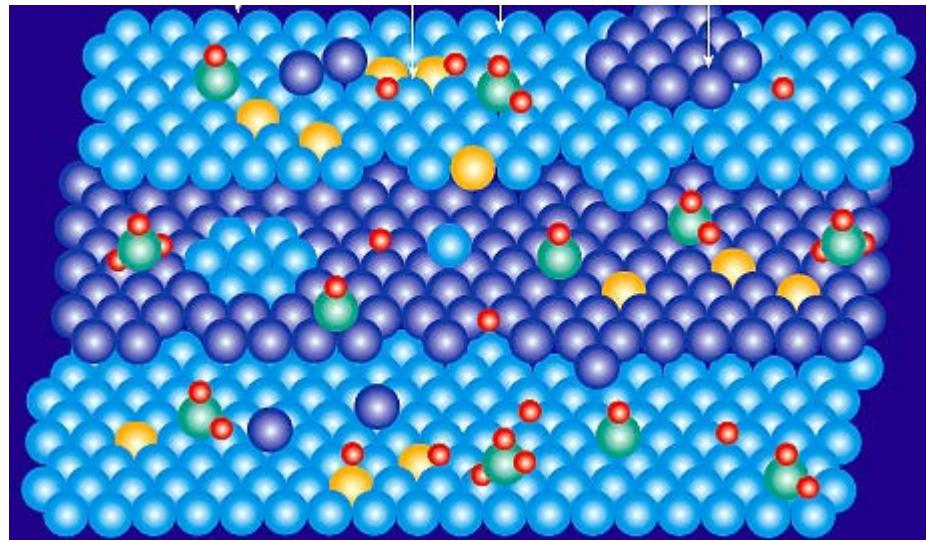
Use quantitative calculations to determine
rate constants and test reaction mechanisms



The effective site to atomistic gap

*

vs.



Generic active site

Independent of operation conditions

One site model

Atomistic active site model

Every atom counts

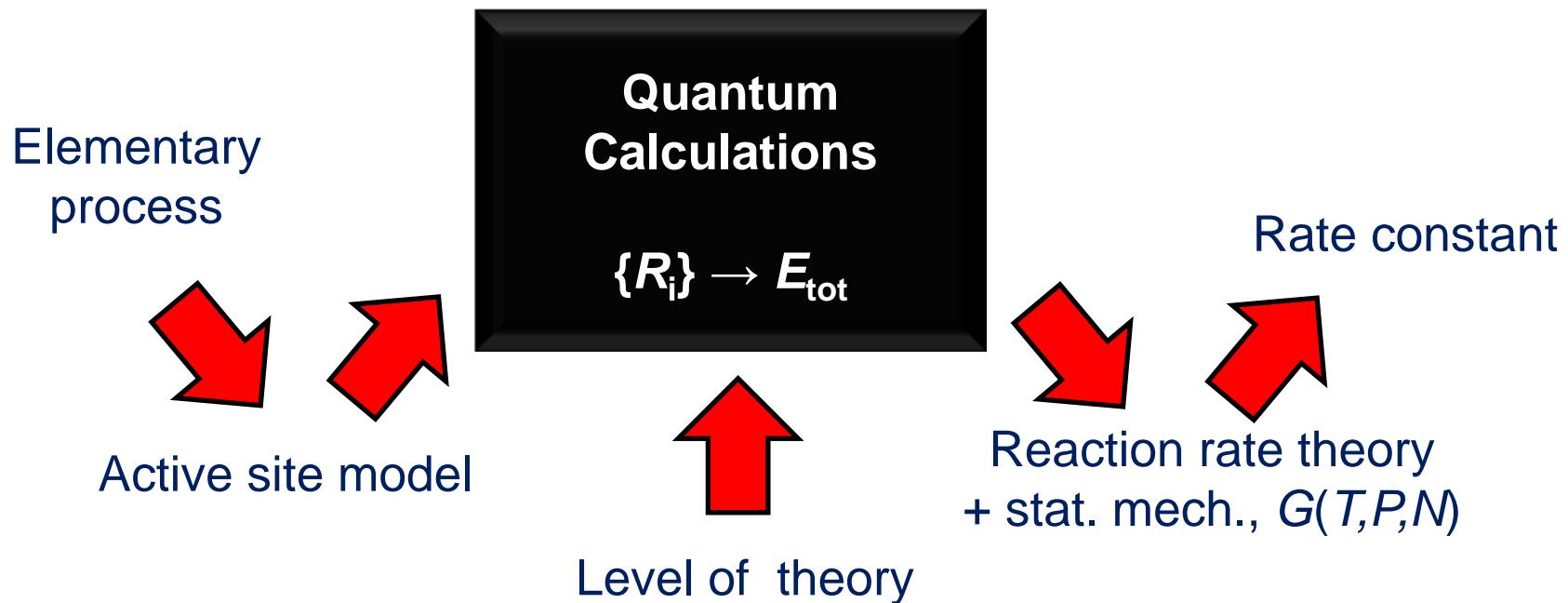
Generally insufficient characterization

Distribution of active site types

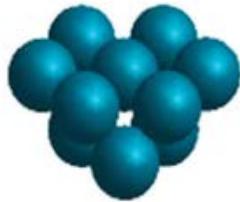
On which one to focus?

Consider how many?

The crucial ingredients toward first-principles microkinetics



Active site models

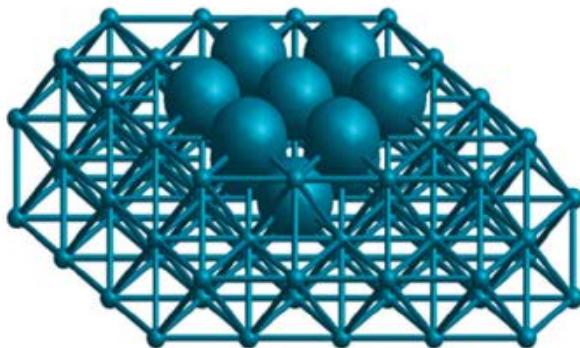


Cluster

Ionic insulators

MgO, zeolites, ...

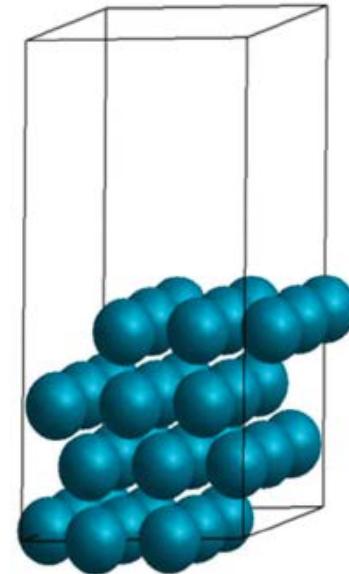
Localized electrons



Embedded Cluster

Non-ionic insulators

TiO₂, Al₂O₃, ...



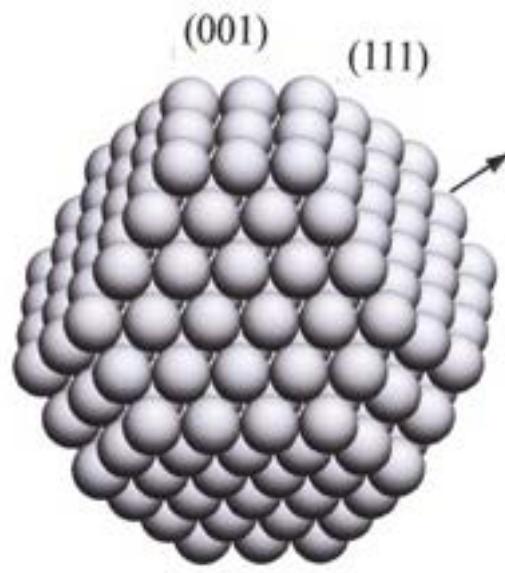
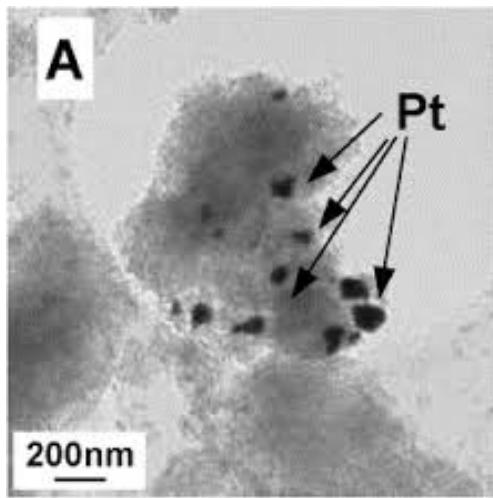
Supercell

Metals or metal-oxides

Pt, Pd, RuO₂...

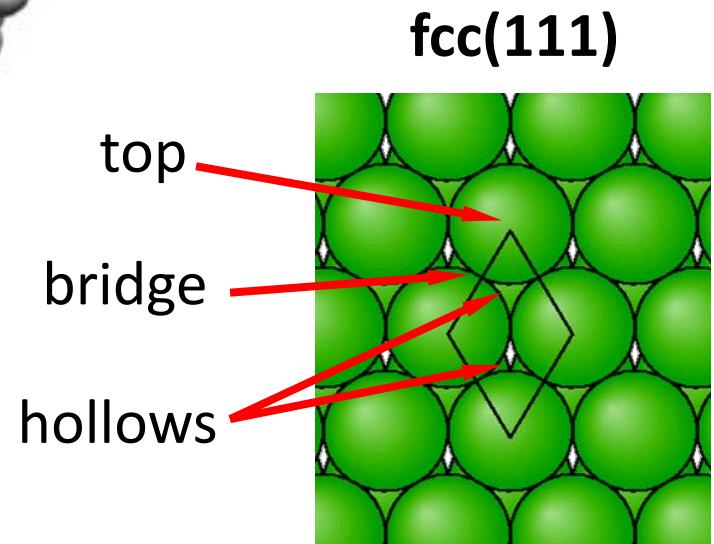
Use periodic boundary conditions
to capture metallic band structure

Simple examples of active site models

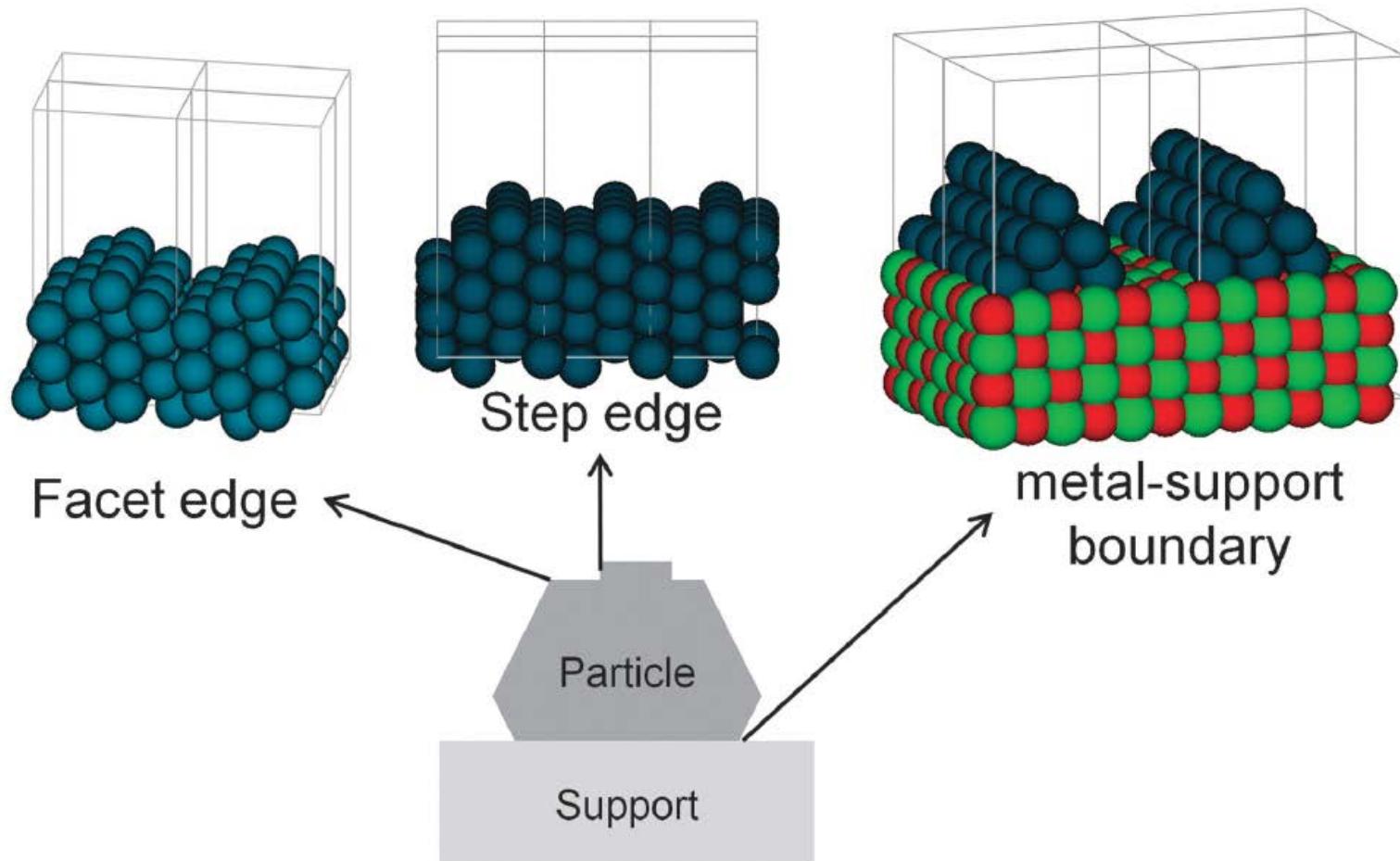


Theoretical
surface science approach

Neglect facet edge effects
Assume ideal terraces



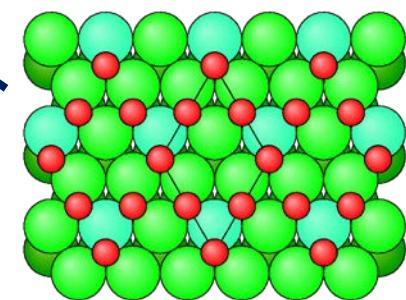
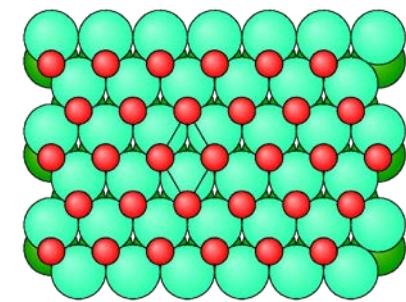
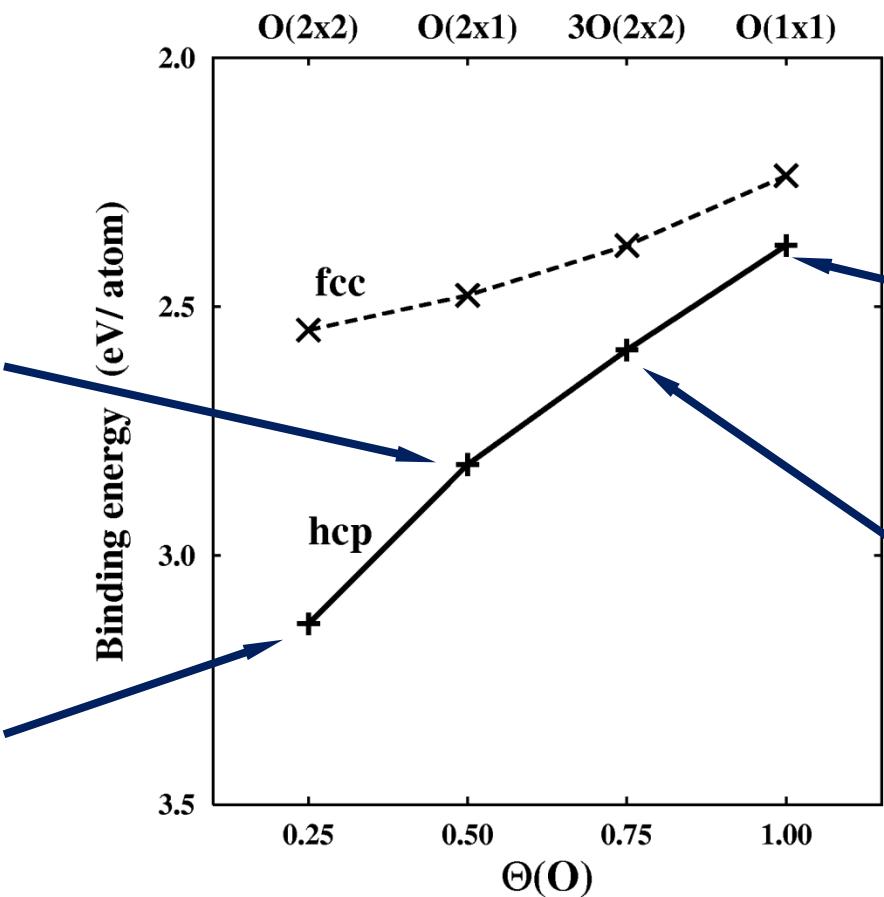
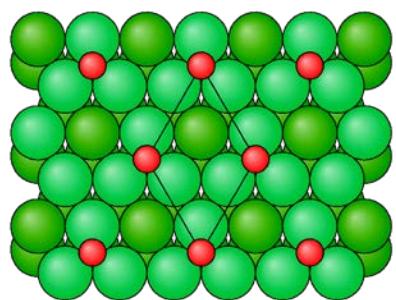
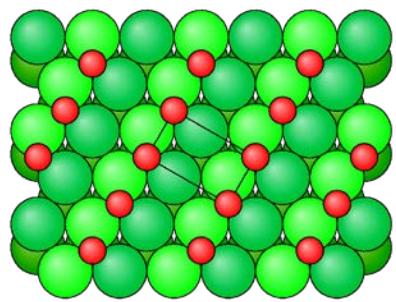
More advanced examples of active site models



Thermochemical calculations: Adsorption sites, lateral interactions, desorption enthalpies

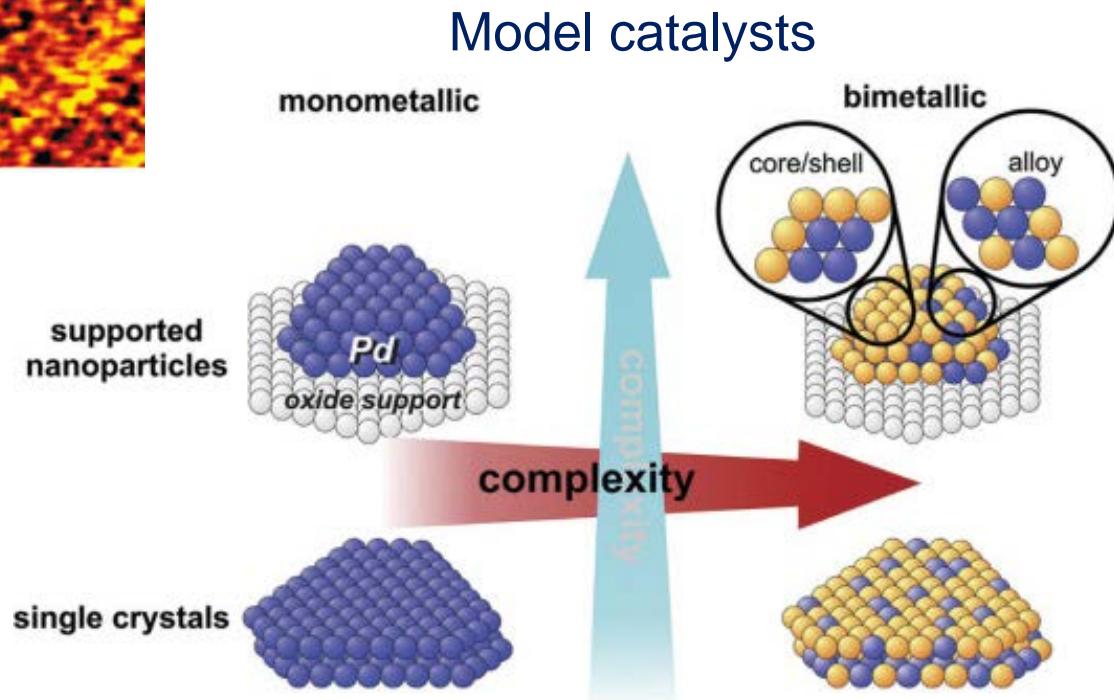
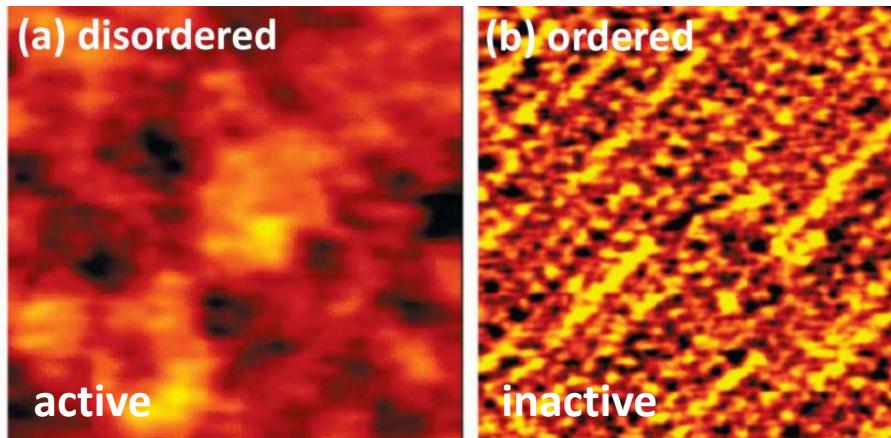
$$E_{\text{binding}} = - \left[E^{\text{tot}} \left(\begin{array}{c} \text{red sphere} \\ \hline \text{green hatched surface} \end{array} \right) - E^{\text{tot}} \left(\begin{array}{c} \text{green hatched surface} \\ \hline \text{green hatched surface} \end{array} \right) - \frac{1}{2} E^{\text{tot}} \left(\begin{array}{cc} \text{red sphere} \\ \text{red sphere} \end{array} \right) \right]$$

Oxygen adsorption
on Ru(0001)



Mind the materials gap!

STM images during high pressure ethylene hydrogenation on Rh(111)



Real vs. model materials: The materials and pressure gaps

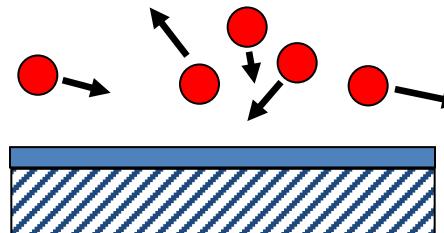
A DFT calculation corresponds to $T = 0 \text{ K}$

Real materials may be full of defects (vacancies, dislocations, dopants)

Material's structure and composition can strongly depend on preparation

Impurities and adsorbates can influence the surface morphology

A surface cannot be separated from a gas (or liquid) above it



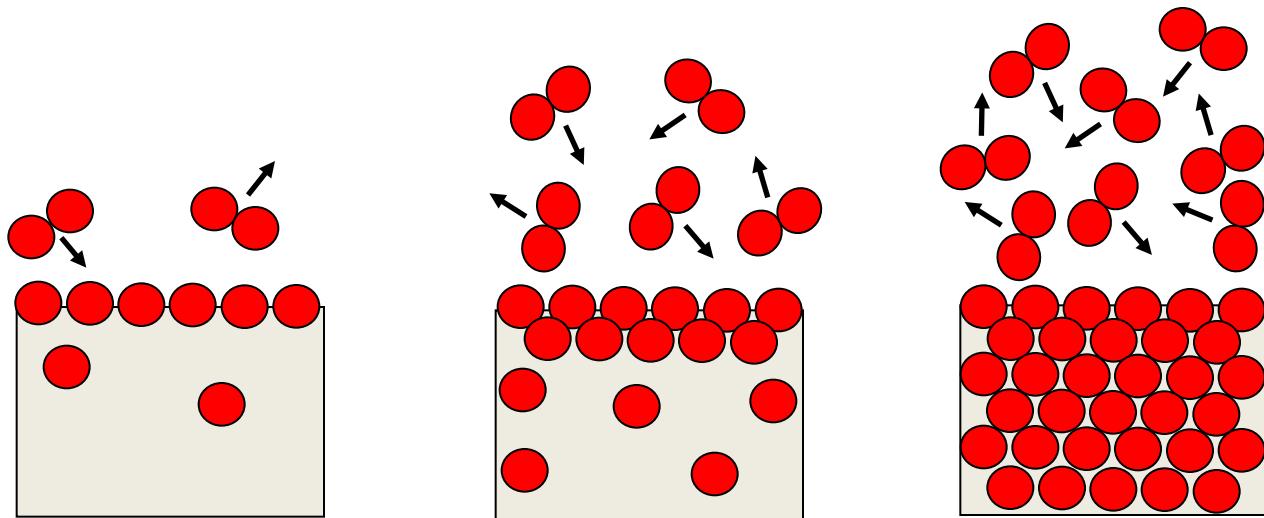
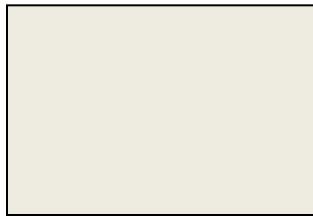
$$v = \frac{p}{\sqrt{2\pi mkT}}$$

Requires $p \leq 10^{-12} \text{ atm}$ to
keep a “clean” surface clean

For $T = 300 \text{ K}$, $p = 1 \text{ atm}$

$$v \approx 10^8 \text{ site}^{-1} \text{ s}^{-1}$$

Bridging the pressure and temperature gap

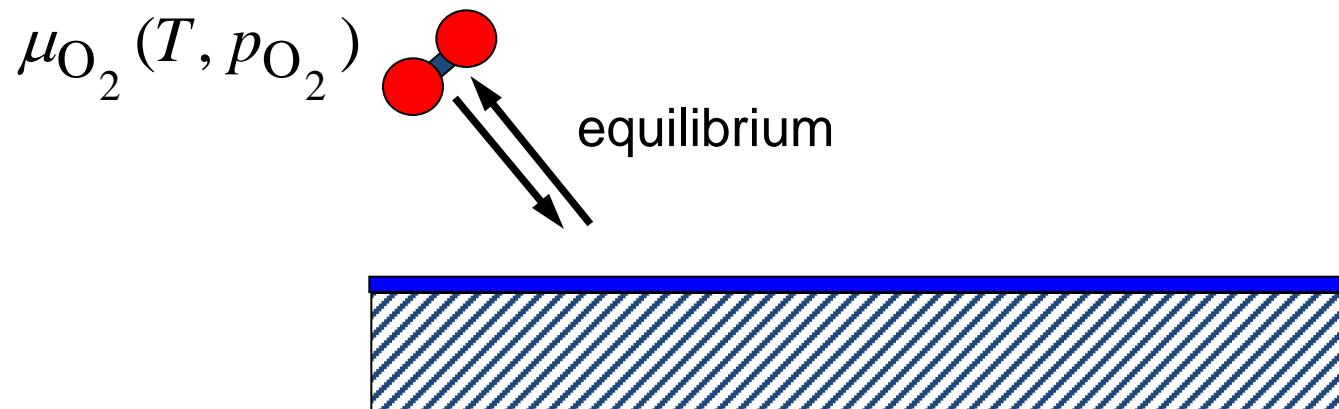


Theory: Development and use of first-principle statistical mechanics approaches → *ab initio* thermodynamics

Experiment: Awareness and diligent experiments...
Development and use of *in situ* techniques

Ab initio thermodynamics provides a connection between the microscopic and macroscopic regimes

Predict the preferred structure of a material as a function of environmental conditions



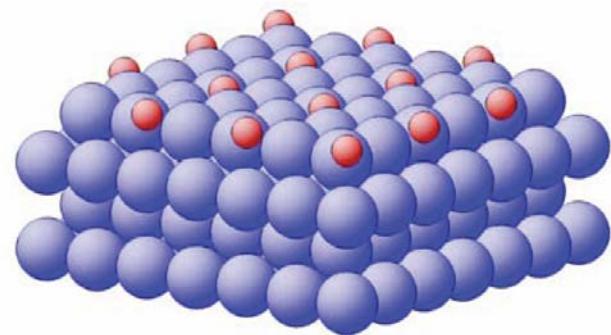
$$G(T, p) = E^{\text{total}} + F^{\text{vibration}} - TS^{\text{configurational}} + pV$$

DFT

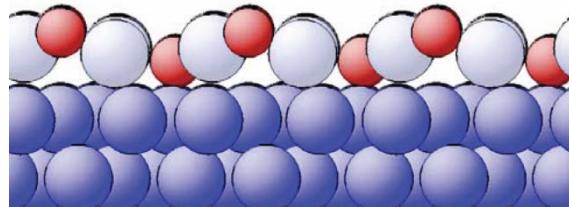
A dotted arrow points from the text "DFT" to the term E^{total} in the equation.

- [1] C.M. Weinert and M. Scheffler, *Mater. Sci. Forum* 10-12, 25 (1986)
- [2] G.-X. Qian, R.M. Martin, and D.J. Chadi, *Phys. Rev. B* 38, 7649 (1988)
- [3] K. Reuter and M. Scheffler, *Phys. Rev. B* 65, 035406 (2002)

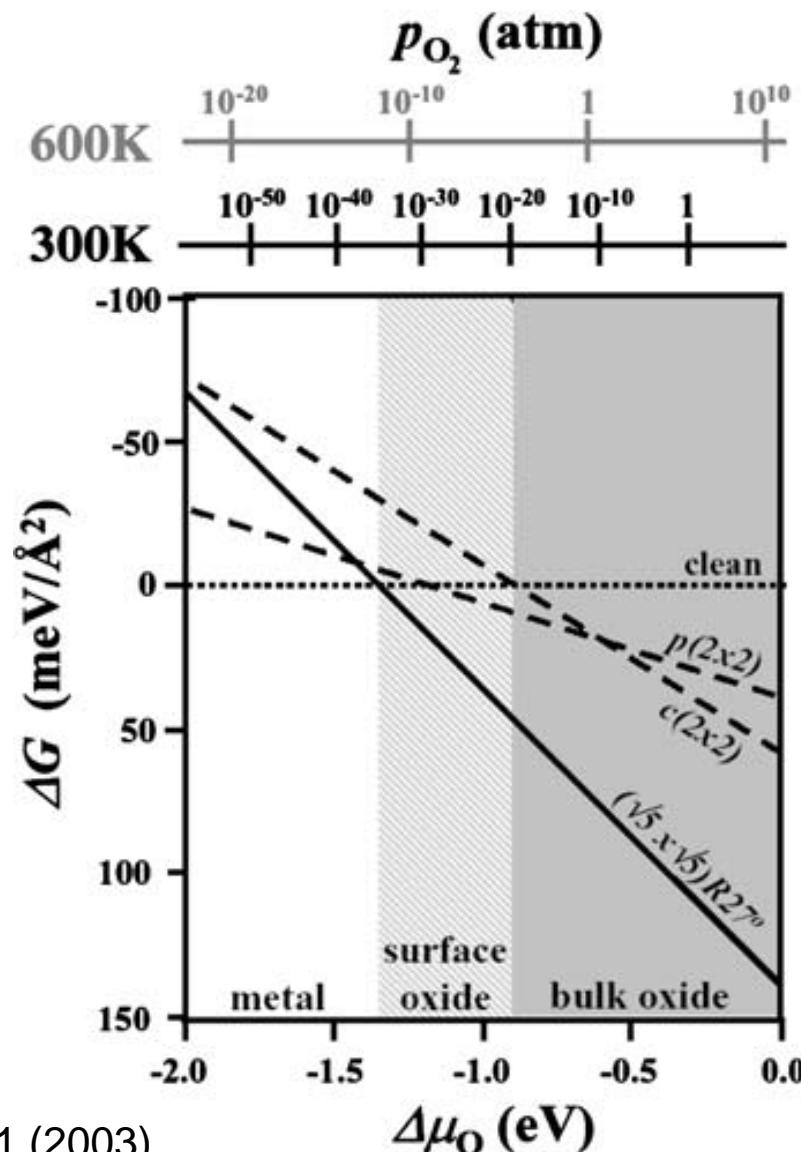
Example of *ab initio* thermodynamics: Pd(100) metal surface in contact with O₂ gas



$p(2\times 2)$ O/Pd(100)



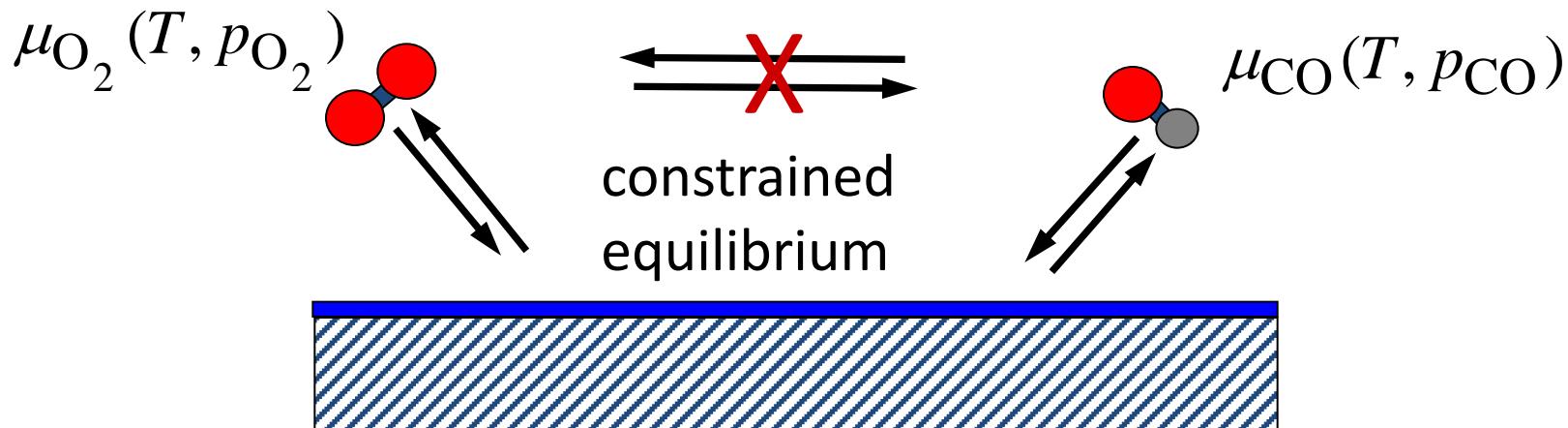
$(\sqrt{5}\times\sqrt{5})R27^\circ$ PdO(101)/Pd(100)



[1] M. Todorova *et al.*, *Surf. Sci.* 541, 101 (2003)

[2] K. Reuter and M. Scheffler, *Appl. Phys. A* 78, 793 (2004)

Ab initio thermodynamics: constrained equilibria

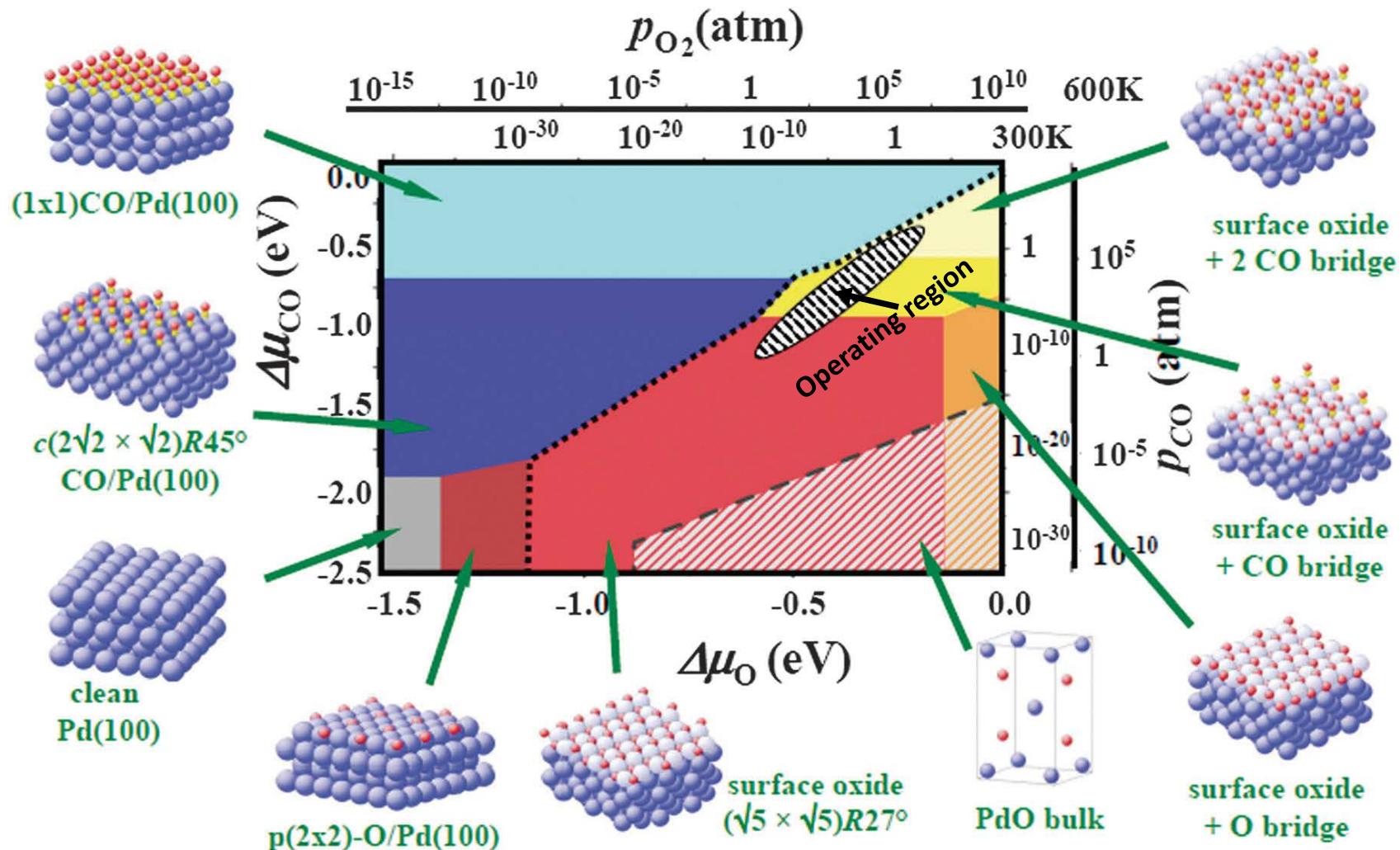


$$G(T, p) = E^{\text{tot}} + F^{\text{vib}} - TS^{\text{conf}} + pV$$

DFT

- [1] C.M. Weinert and M. Scheffler, *Mater. Sci. Forum* 10-12, 25 (1986)
- [2] E. Kaxiras *et al.*, *Phys. Rev. B* 35, 9625 (1987);
- [3] K. Reuter and M. Scheffler, *Phys. Rev. B* 65, 035406 (2001)

Surface phase diagram for the Pd(100) surface with an environment consisting of O₂ and CO



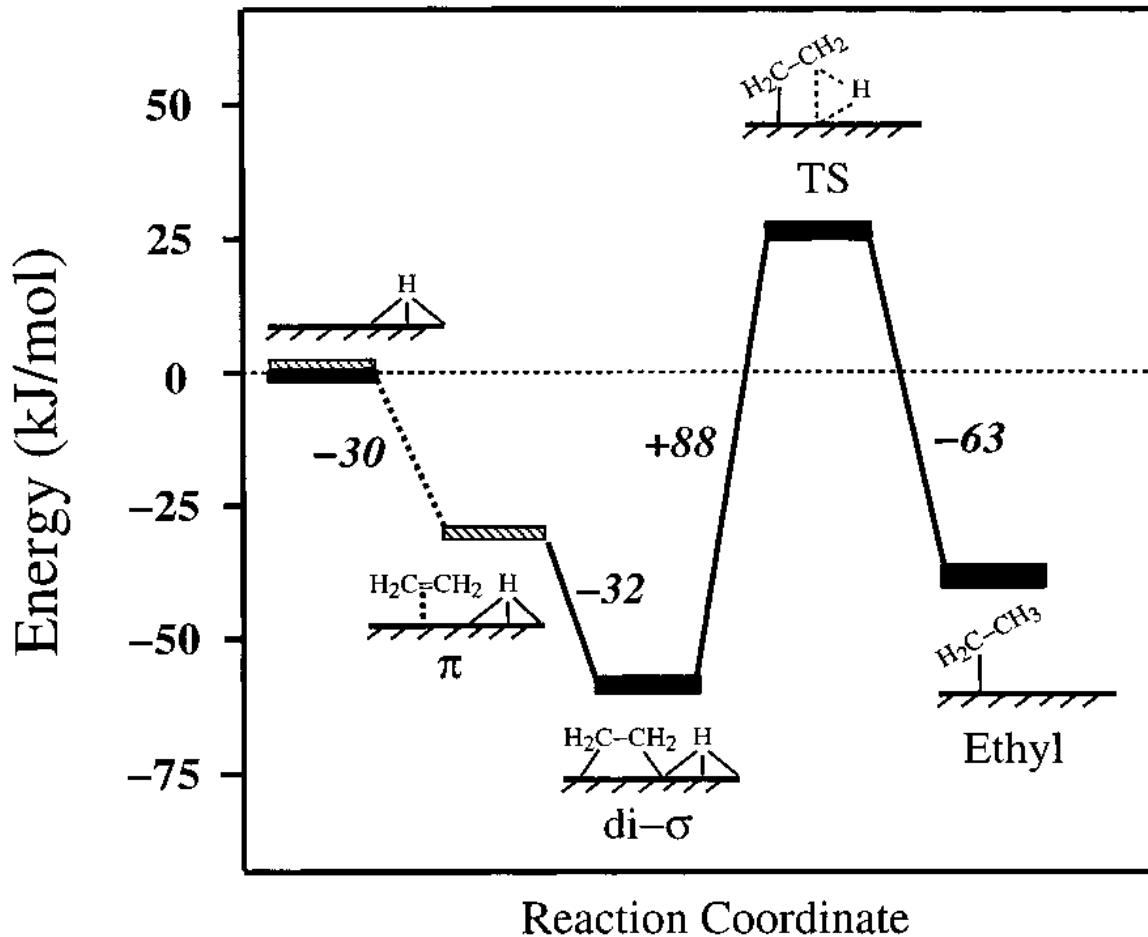
Pd: large blue spheres, O: small red spheres, C: white spheres

[1] K. Reuter and M. Scheffler, *Phys. Rev. Lett.* 90, 4 (2003)

[2] J. Rogal, K. Reuter, M. Scheffler, *Phys. Rev. Lett.*, 98, 046101 (2007)

Understanding reactions on surfaces: Potential energy diagrams

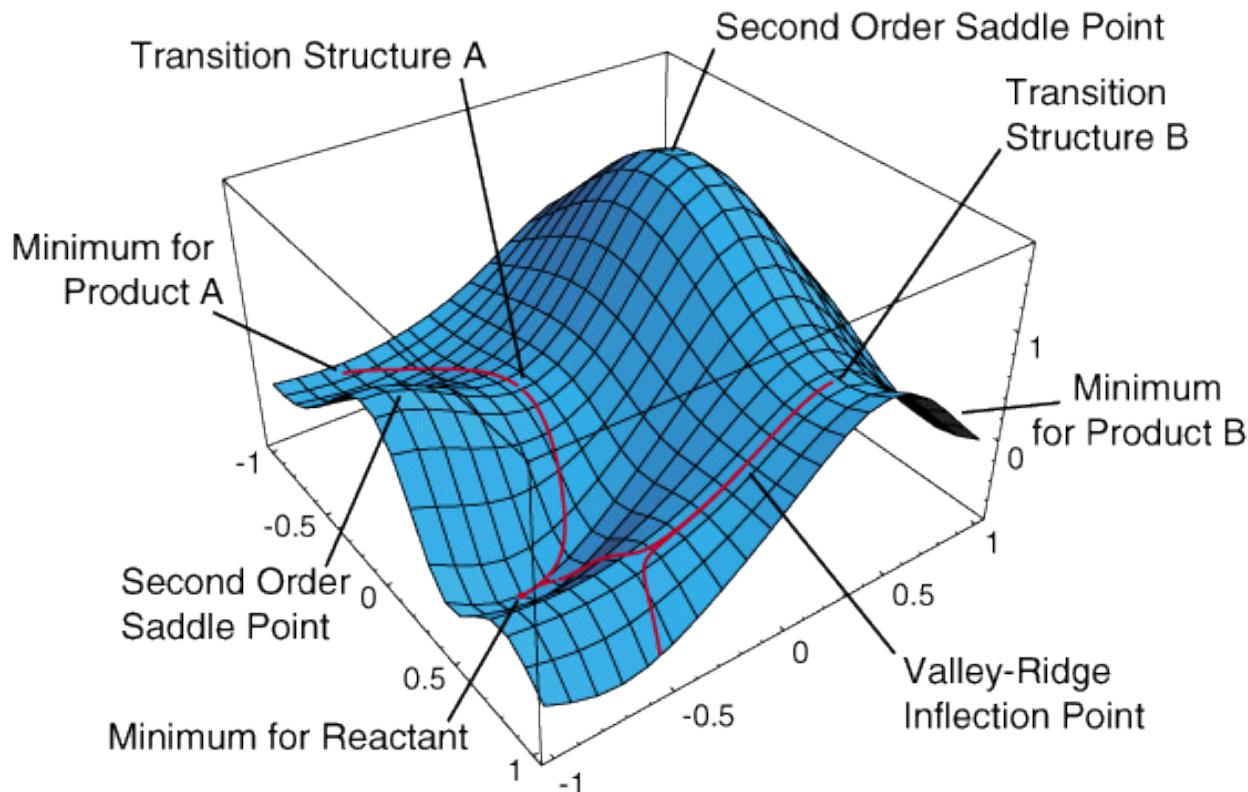
Ethene hydrogenation to a surface ethyl intermediate on Pd(111)



Potential energy diagrams amount to finding the relevant minima and transition states for a given reaction

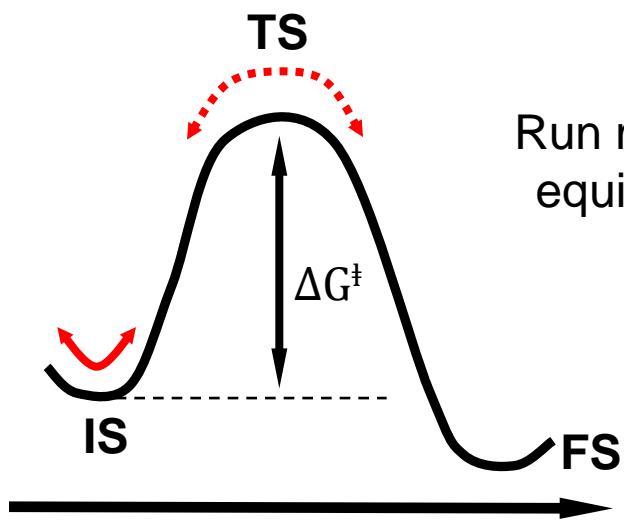
Potential Energy Surface (E, R_i)

($3N+1$) dimensional



Knowledge of the minima and transition states
enables the estimation of reaction rates

Reaction rate theory: Rare event dynamics



Brute force approach to rate constants

Run molecular dynamics trajectory so long that it establishes equilibrium, crossing the barrier many times back and forth

$$k = \frac{\text{no. of crossings IS} \rightarrow \text{FS per unit time}}{\text{fraction of time system has spent in IS}}$$

Relevant time step in molecular dynamics simulation is fs (molecular vibrations)
Typical barrier ΔG^\ddagger for surface reactions $\sim 1 \text{ eV} \Rightarrow 10^{-2} - 10^2$ reactions per second

Requires to run trajectory about $10^{15} - 10^{20}$ time steps \rightarrow **unfeasable...**
...and essentially 99.9% of the time the system will just vibrate in IS basin.

**Requires approximate theories to obtain process rates
(or accelerated sampling methods)**

Transition state (activated complex) theory

(Eyring, Evans, Polanyi, ~1935)

Assumptions

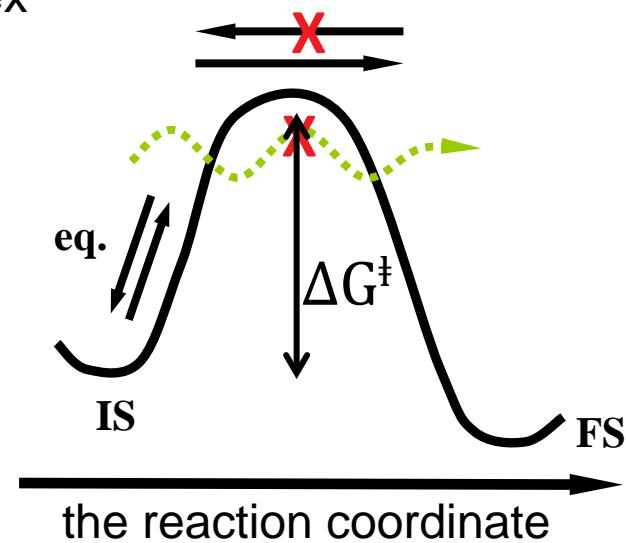
Reacting system passes over the barrier top only once (no recrossings)

Energy distribution of reactant degree of freedom (DOF) is Boltzmann-like

Passage over barrier is the motion of only one DOF, *the reaction coordinate*, which is independent of all other motions of the activated complex

Passage over barrier is a classical event (no tunneling)

$$k = \frac{k_B T}{h} \exp\left(-\frac{\Delta G^\ddagger}{k_B T}\right)$$



problem reduces to locating transition states,
i.e., 1st order saddle points on the potential energy surface

Transition state search algorithms: Nudged Elastic Band

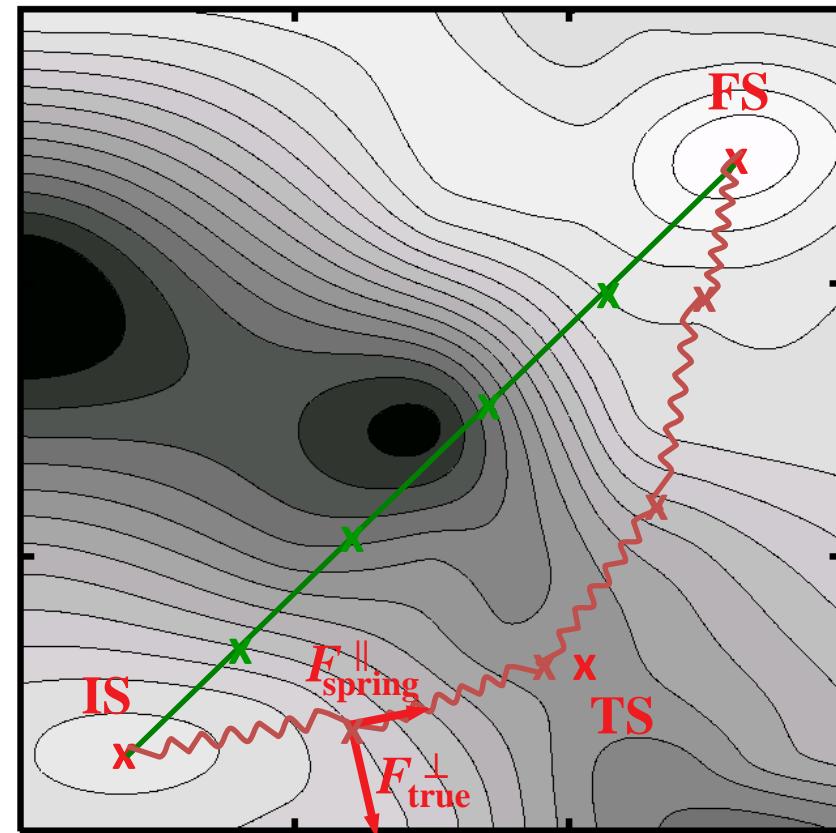
NEB is a widely applied workhorse for finding transition states on surfaces

Initialize with several images $\{R_i\}$ along a straight-line interpolation from IS to FS

$$\text{Minimize } S(R_1, \dots, R_N) = \sum_i E(R_i) + \sum_i k/2 (R_{i+1} - R_i)^2$$

only spring force component parallel to path (no corner cutting)

only true force component perpendicular to path (no down-sliding)



[1] G. Mills and H. Jónsson, *Phys. Rev. Lett.* 72, 1124 (1994)

[2] G. Henkelman and H. Jónsson, *J. Chem. Phys.* 113, 9978 (2000)

Transition state search algorithms: Dimer method

Initialize by putting a dimer^[1] (two similar images) near a guessed transition state

Rotate dimer to minimize energy
(along direction of lowest frequency mode)

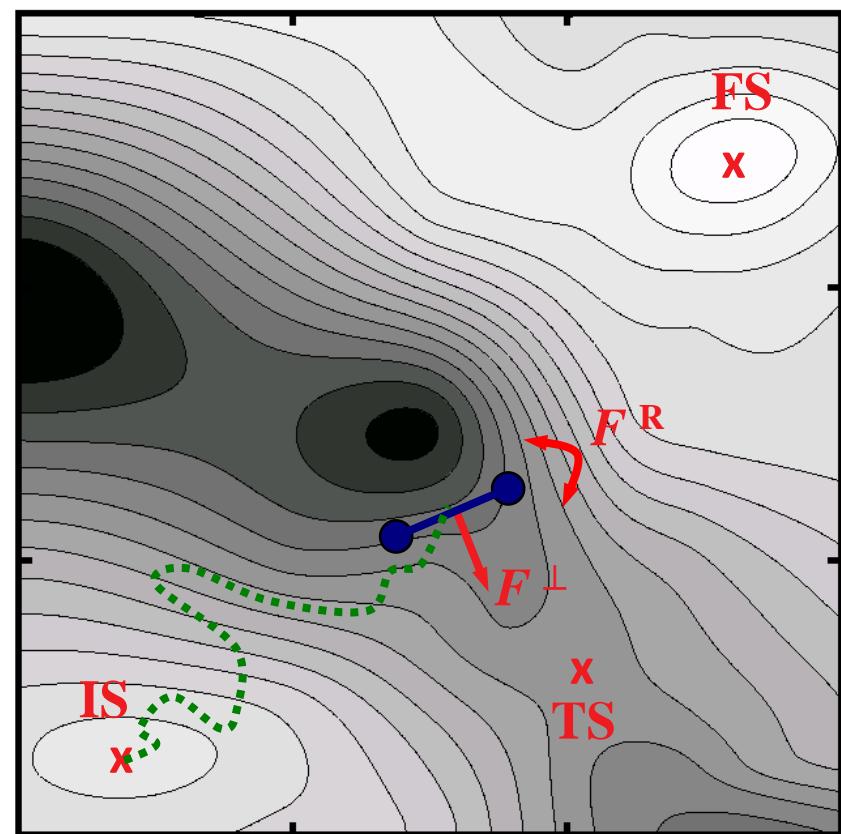
Move dimer along gradient \perp to dimer axis

Advantage

- works without any information about FS
- can discover unexpected transition states

Generally

- no algorithm is fool-proof
- still room for new ideas

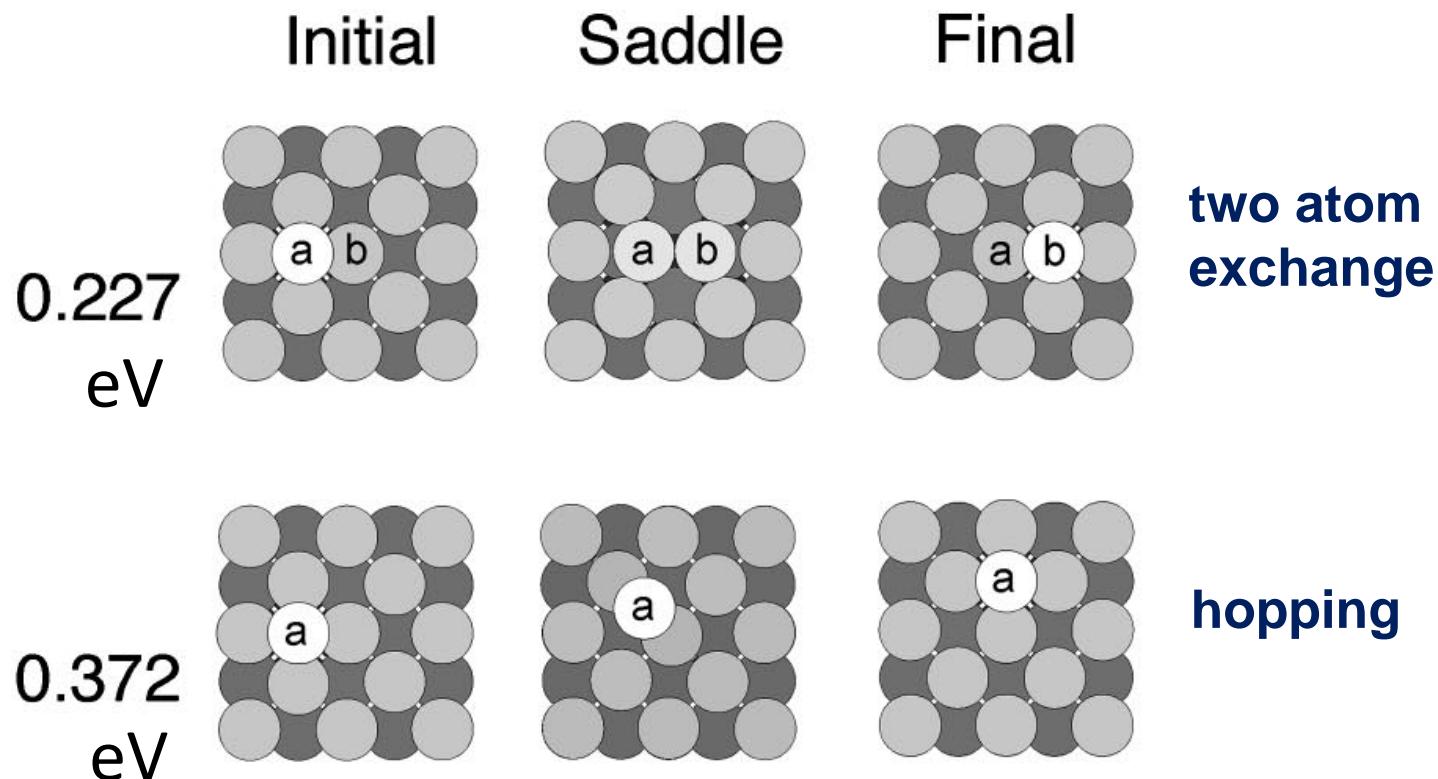


[1] G. Henkelman and H. Jónsson, *J. Chem. Phys.* 111, 7010 (1999)

Identifying the Processes...

Diffusion at metal surfaces: surprises...

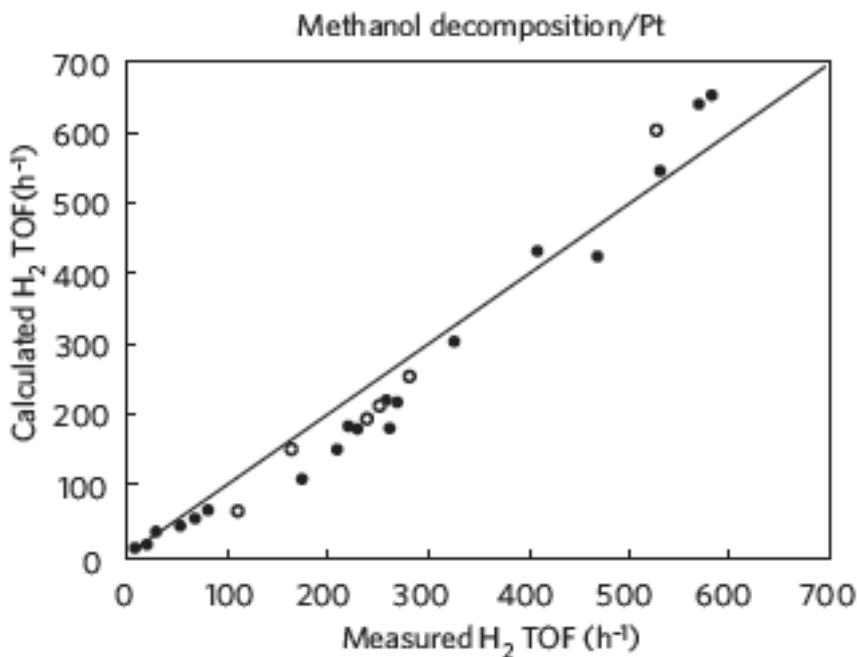
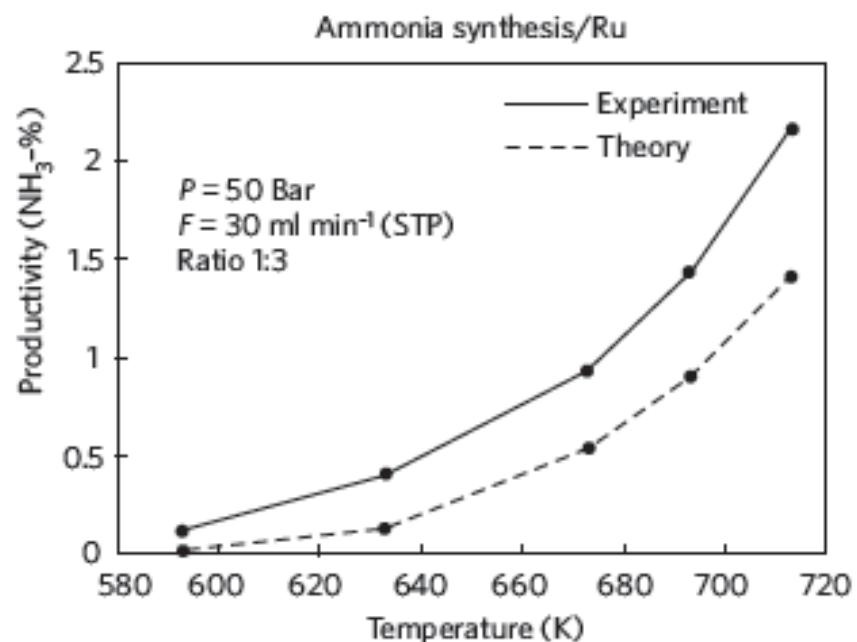
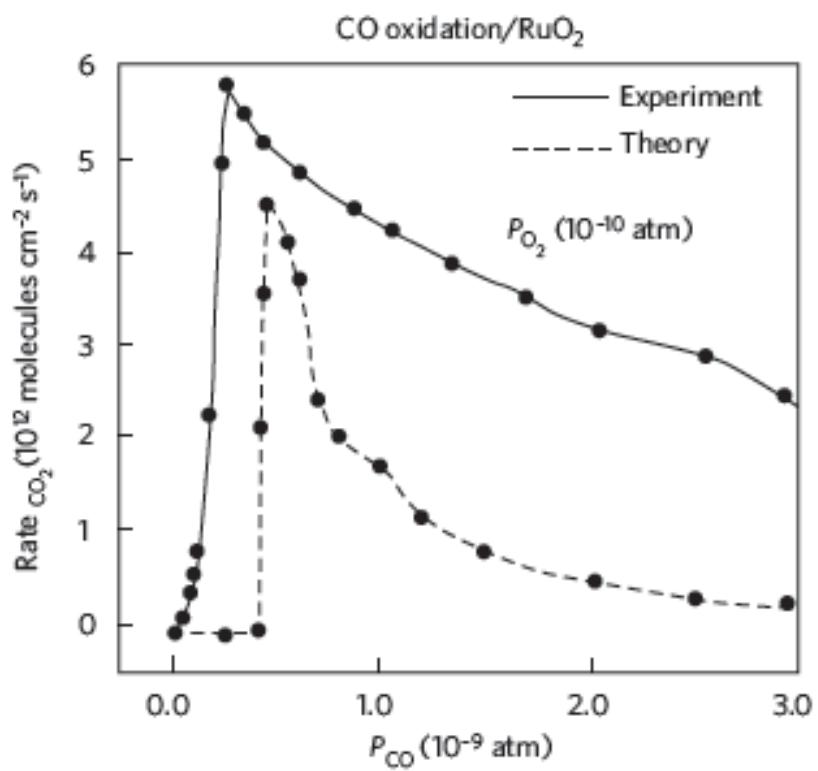
Al adatom is initially sitting in the fourfold hollow site on Al(100) surface



10 minutes for stretching, restroom, water, etc



The dawn of a new era



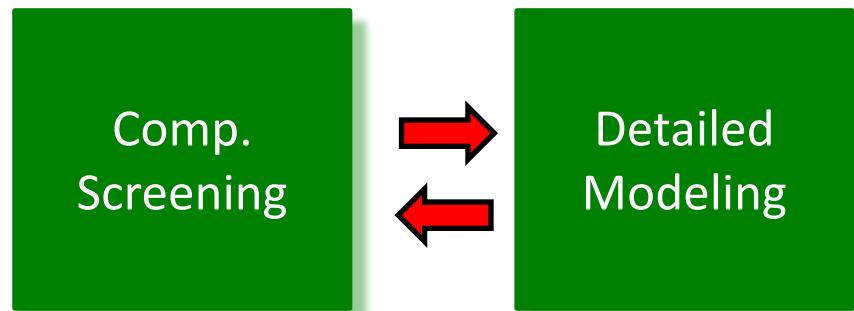
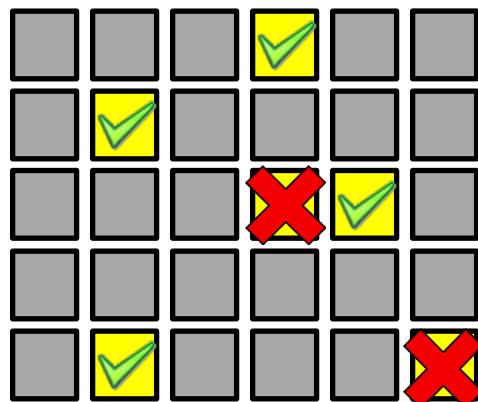
Computational screening: Think inaccurate!

Good descriptor is necessary

The cheaper the descriptor, the more screening

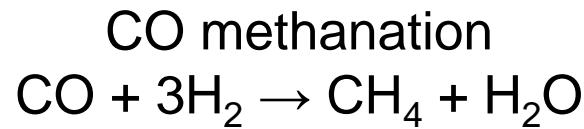
The better the descriptor,
the more meaningful the results

Multi-dimensional descriptors (data mining...)

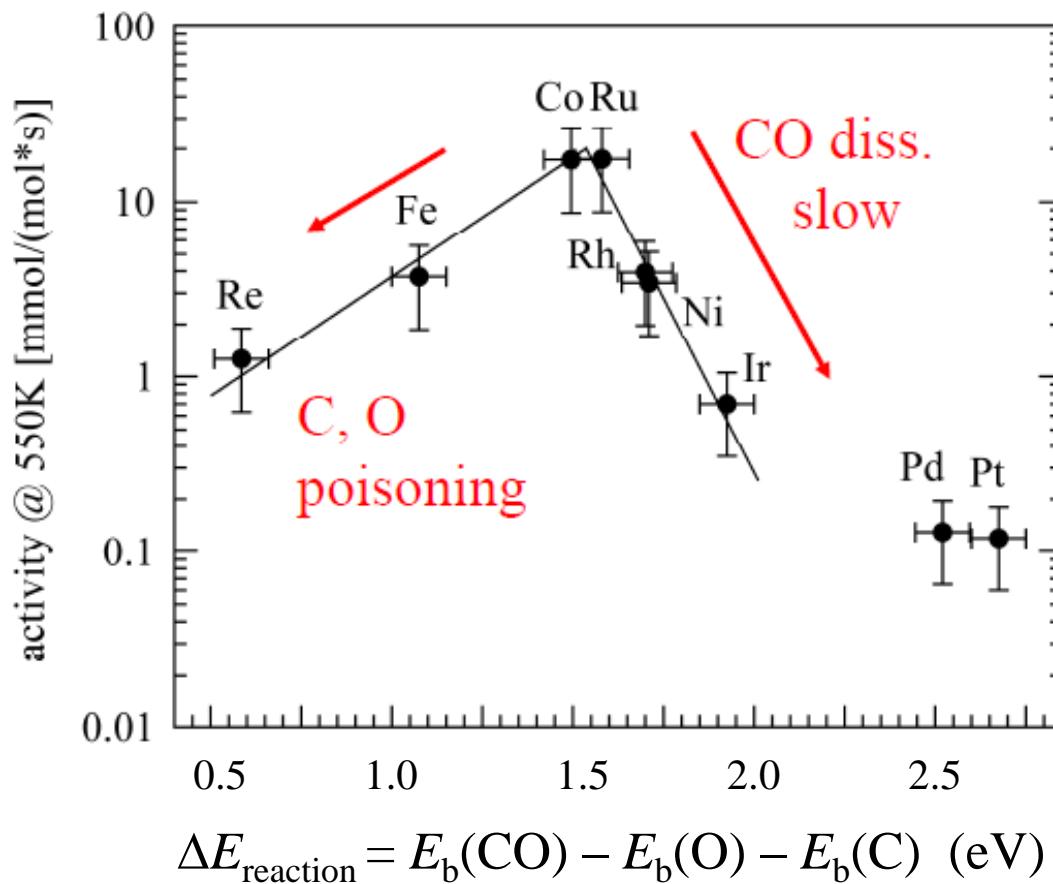


Trends require lower accuracy

Rate-determining step barrier as descriptor: Volcanos



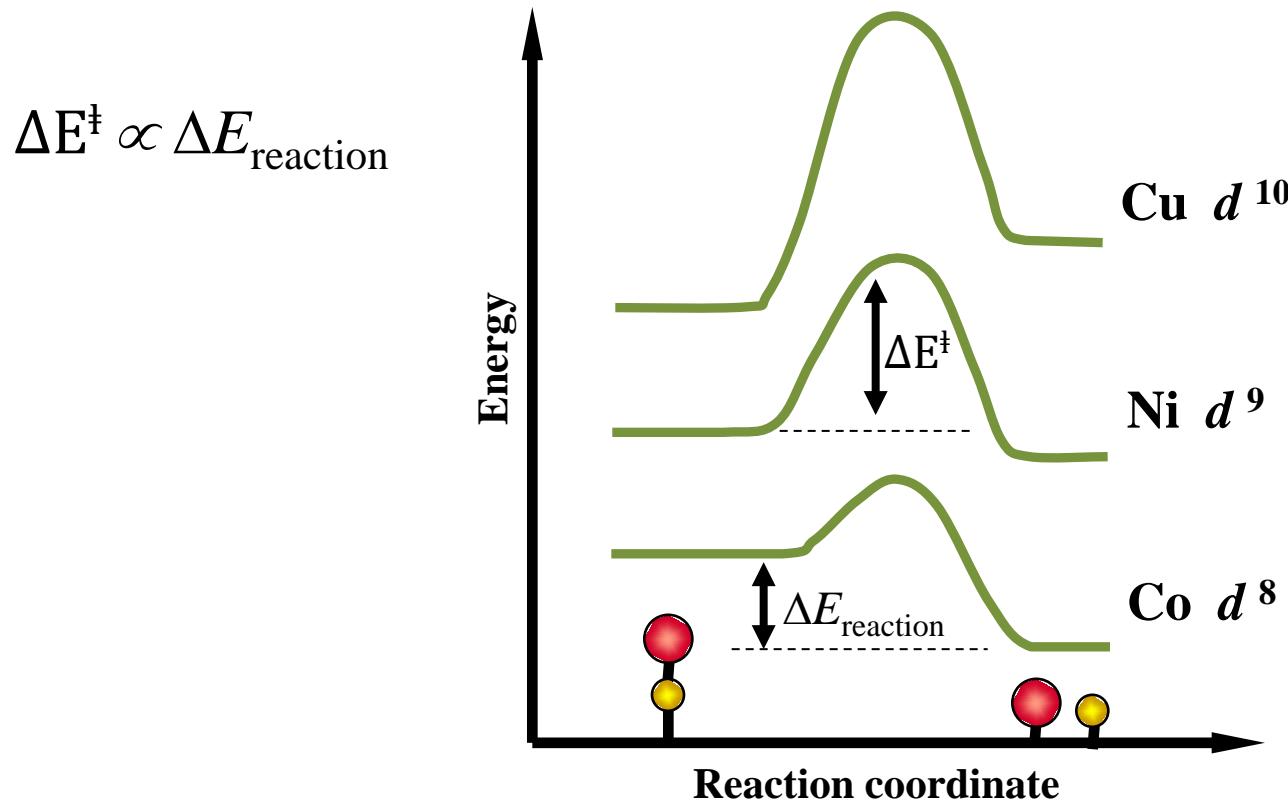
Lower barrier = better,
however, if too low, switch of RDS



Estimating activation barriers: Brønsted-Evans-Polanyi (BEP) relations

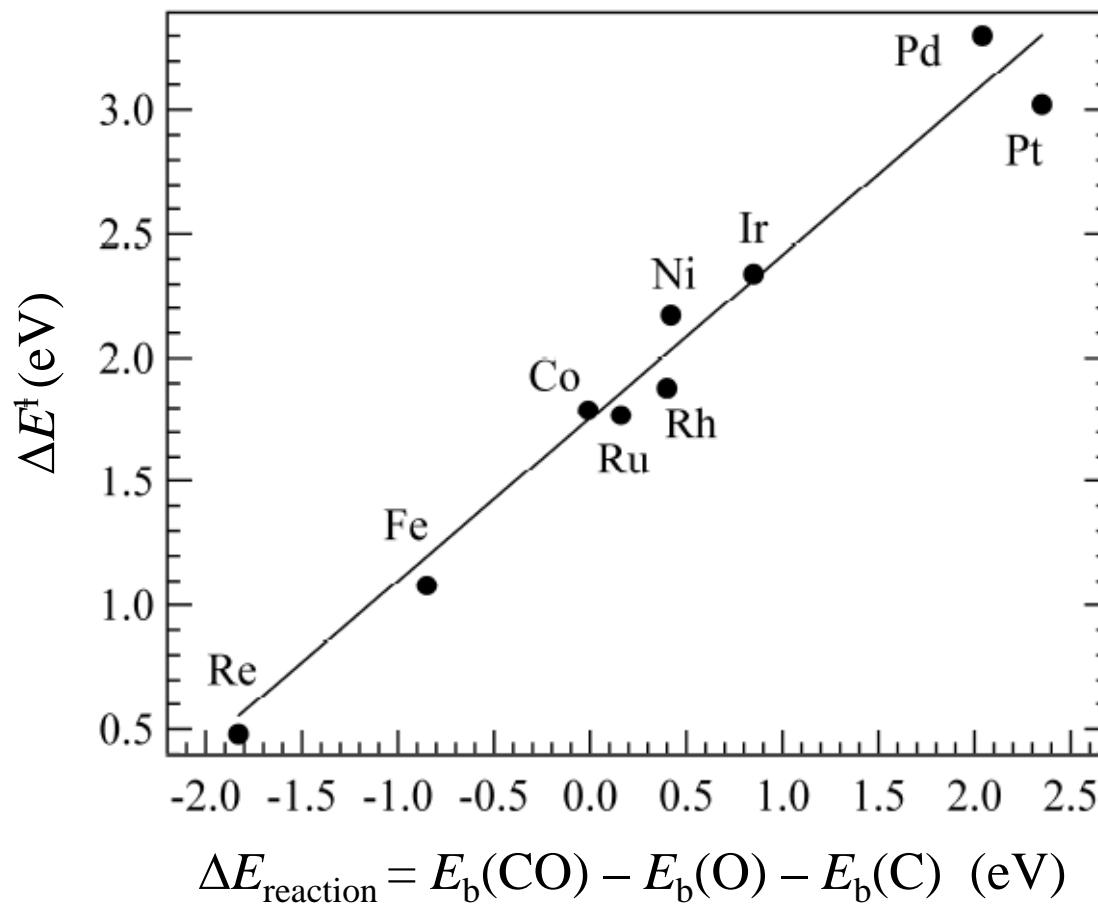
Reaction barriers are tedious to compute

Use as descriptors other easier to compute quantities that relate to the barrier



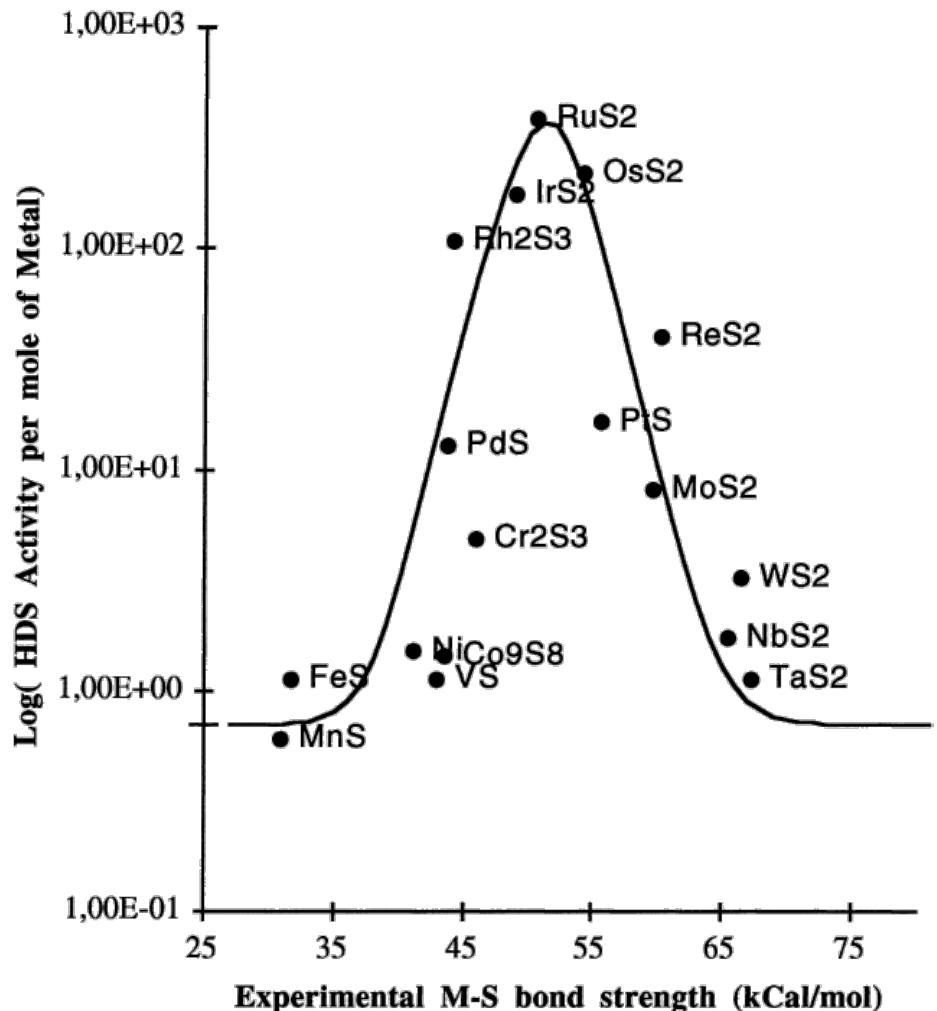
$\Delta E_{\text{reaction}}$ here related to binding energy of CO, C, O (reaction intermediates).
If BEP relation fulfilled, could use thermochemical data as descriptor.

Brønsted-Evans-Polanyi relation for CO methanation



$E_b < 0$ for exothermic binding

Sabatier principle: The relevance of intermediate bond strength

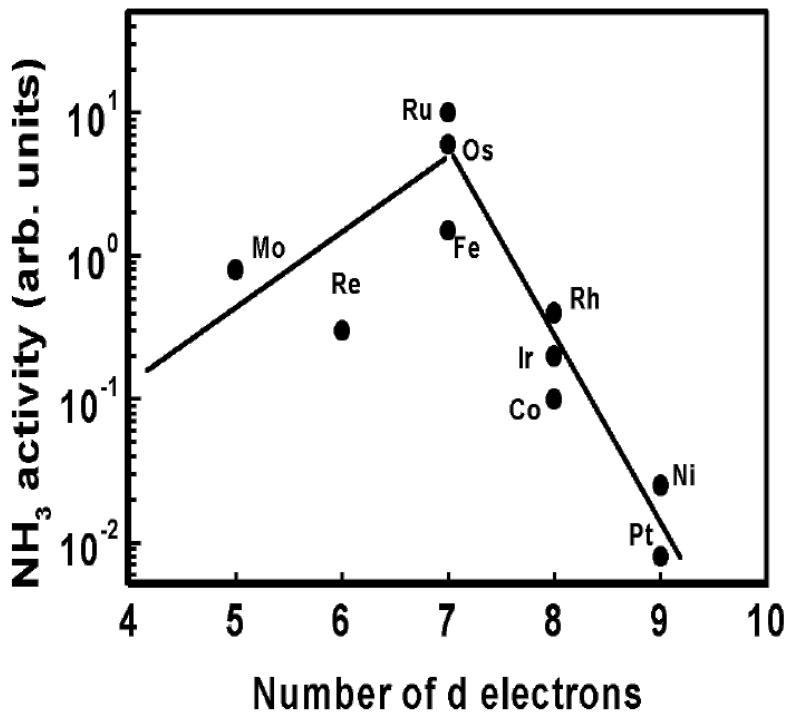


hydrodesulfurization of dibenzothiophene

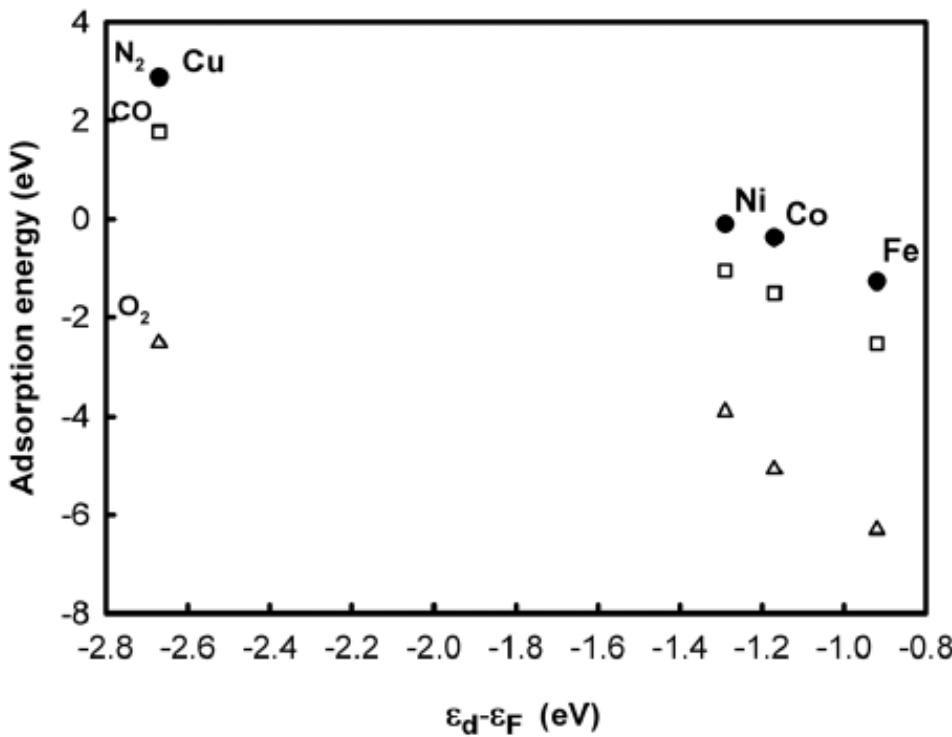
H. Toulhoat *et al.*, Catal. Today 50, 629 (1999)

Low bond strength: no incentive to form/bind intermediates
High bond strength: no incentive to form products

Even more volcanos: *d*-band model



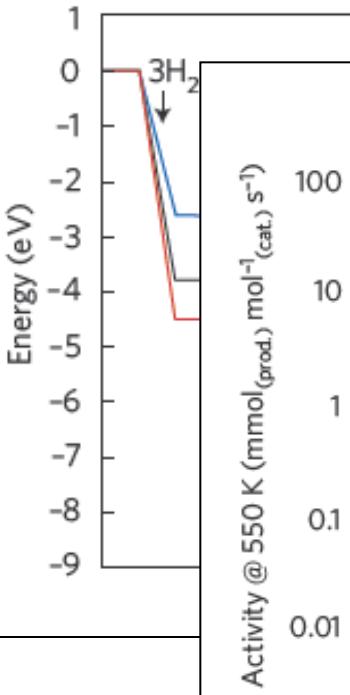
Calculated dissociative nitrogen, carbon monoxide, and oxygen chemisorption energies over different 3d transition metals



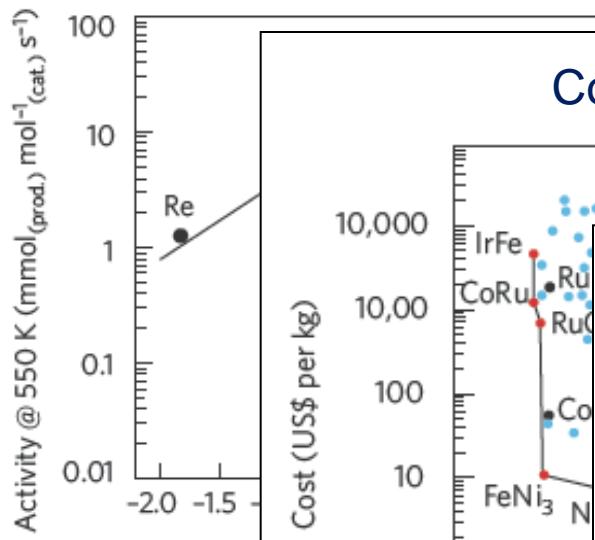
***d*-band position as descriptor**

The vision of rational design

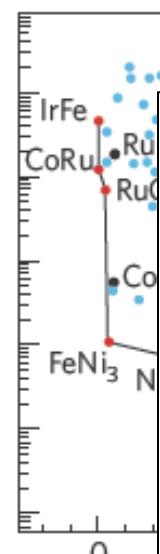
Mechanistic understanding



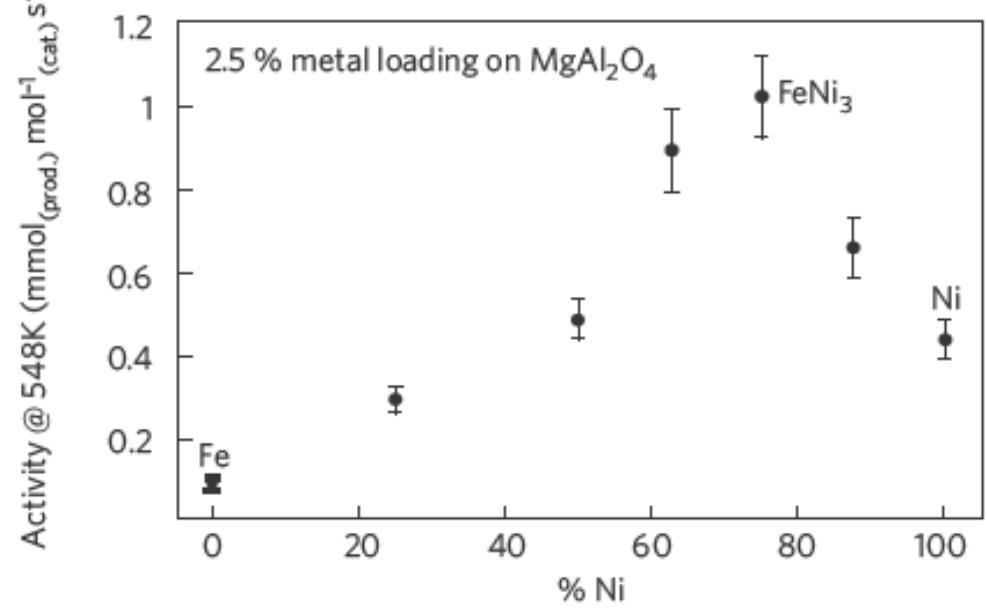
Descriptor



Computational Screening

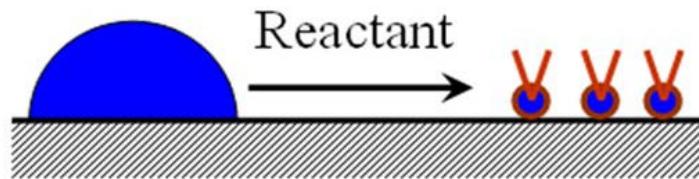


Validation



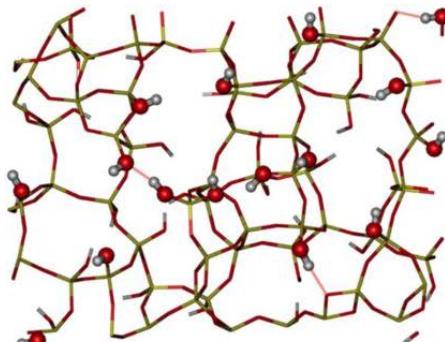
Topical Examples

Disintegration and redispersion of noble metal nanoparticles



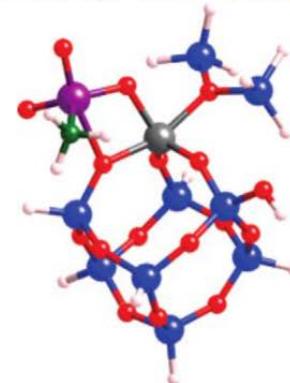
Modeling isolated catalyst sites on amorphous supports

Amorphous oxide
catalysts and supports



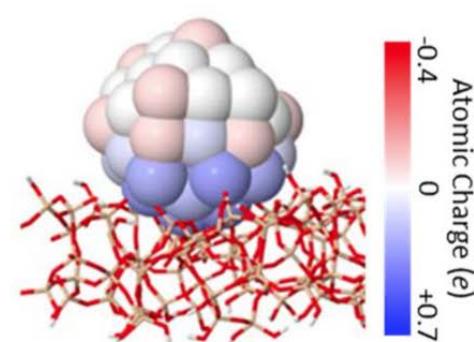
SiO_2

Metals atomically-dispersed
on amorphous supports



$\text{CH}_3\text{ReO}_3 / \text{SiO}_2-\text{Al}_2\text{O}_3$

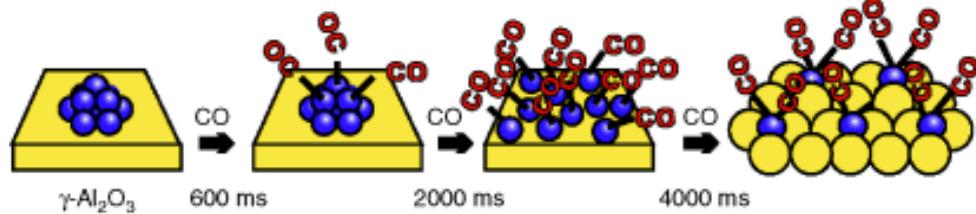
Metal clusters on
amorphous supports



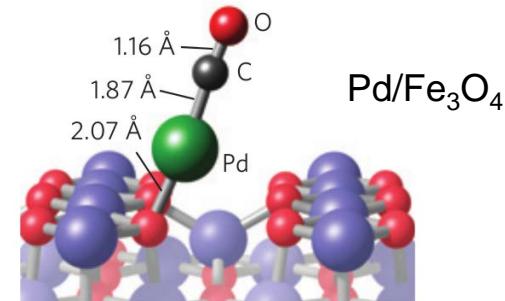
$\text{Pt}_{55} / \text{SiO}_2$

Nanoparticle disintegration can cause catalyst deactivation or change the active site

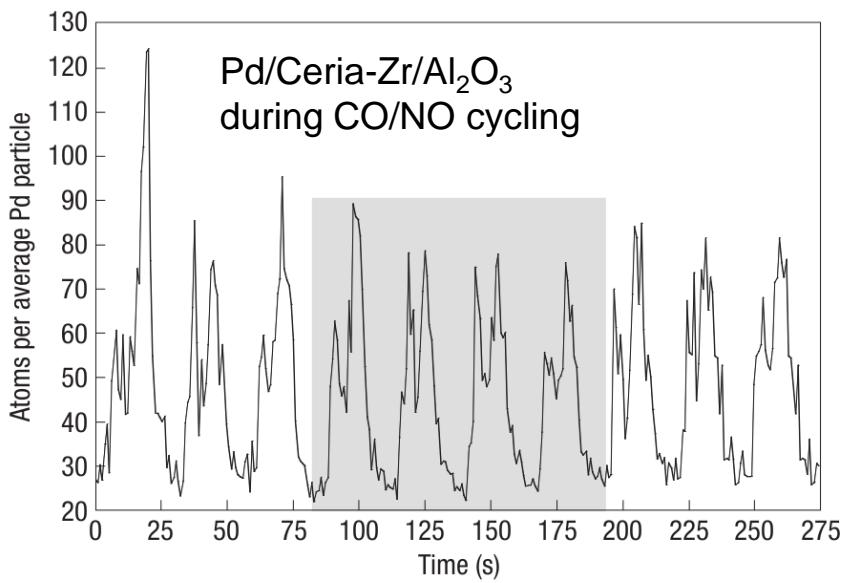
Rh/ Al_2O_3



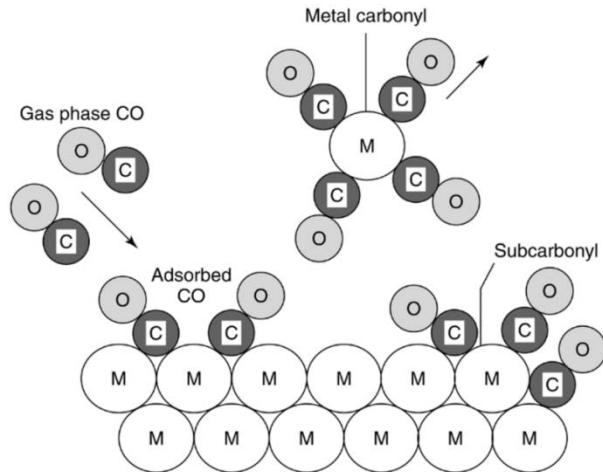
A. Suzuki *et al.*, *Angew. Chem. Int. Ed.* 42 (2003)



G. Parkinson *et al.*, *Nat. Mater.* 12 (2013)

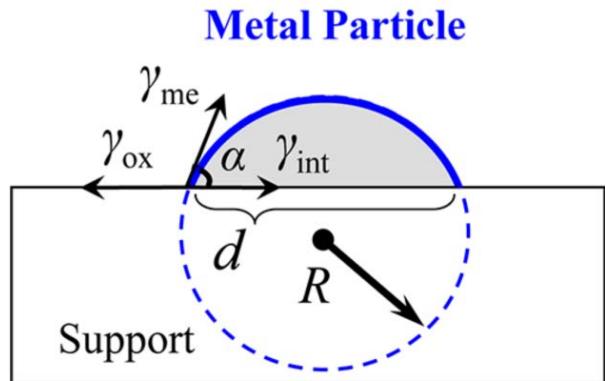


M. Newton *et al.*, *Nat. Mater.* 6 (2007)



M. Argyle and C. Bartholomew, *Catalysts* 5 (2015)

Energetics of supported nanoparticles

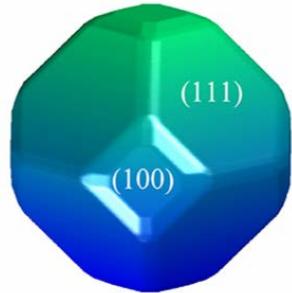


Average energy of particle per atom
with respect to bulk

$$\Delta E_{\text{NP}} = \frac{3\Omega\gamma_{\text{me}}}{R}$$

What about the effect of reactants?

Nanoparticles have
different exposed facets



Wulff constructed Rh particle

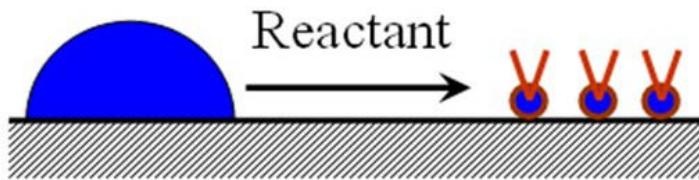
$$\gamma_{\text{me}} = \sum_i f_i \times \gamma_i$$

Surface energy of metal particle ↑
Area ratio of facet i ↑
Surface energy of facet i ↑

- [1] P. Wynblatt, N. A. Gjostein, *Acta Metall.* 24 (1976)
- [2] S. C. Parker, C. T. Campbell, *Phys. Rev. B* 75 (2007)
- [3] R. Ouyang, J.-X. Liu, W.-X. Li, *J. Am. Chem. Soc.* 135 (2013)

Ab initio thermodynamic model for nanoparticle disintegration

$$\Delta G_{\text{disintegration}} < 0$$



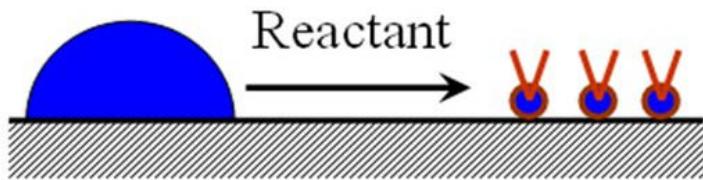
$$\Delta G_{\text{disintegration}}(R, T, p) = G_{\text{adatom-complex}} - G_{\text{reactant}} - G_{\text{nanoparticle}}$$



Free energy for complete
particle disintegration into adatom-complexes

Ab initio thermodynamic model for nanoparticle disintegration

$$\Delta G_{\text{disintegration}} < 0$$



$$\Delta G_{\text{disintegration}}(R, T, p) = E_f - \frac{3\Omega\bar{\gamma}_{\text{me}}}{R} - n \left[\mu_x^0(T, p_0) + k_B T \ln \frac{p_x}{p_0} \right] - TS$$

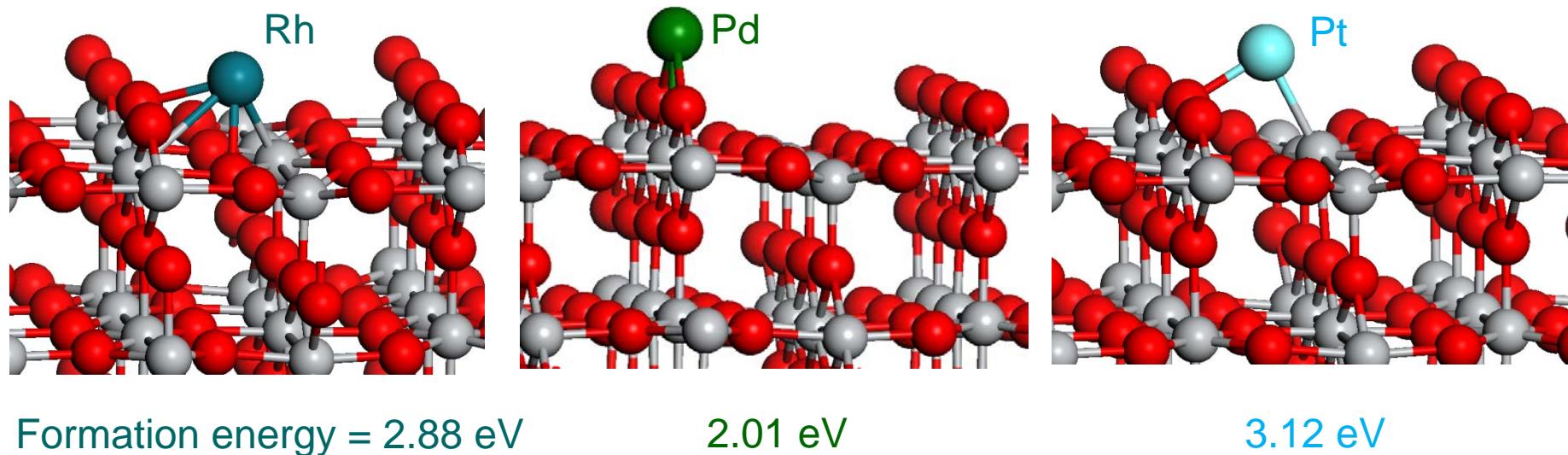
Formation energy of adatom complex

Average energy per atom in NP under reaction conditions wrt. bulk

Standard gas phase chemical potential

Entropy of adatom complexes

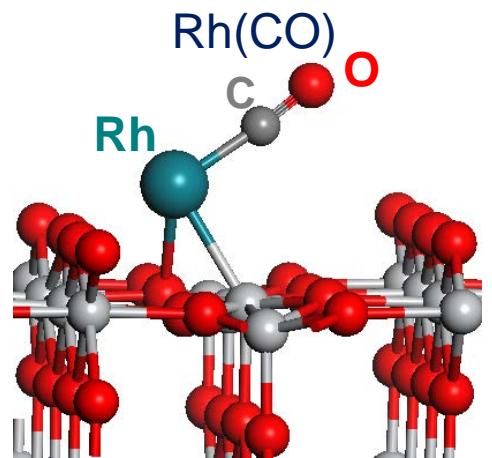
Negligible concentration of bare Rh, Pd and Pt adatoms on $\text{TiO}_2(110)$



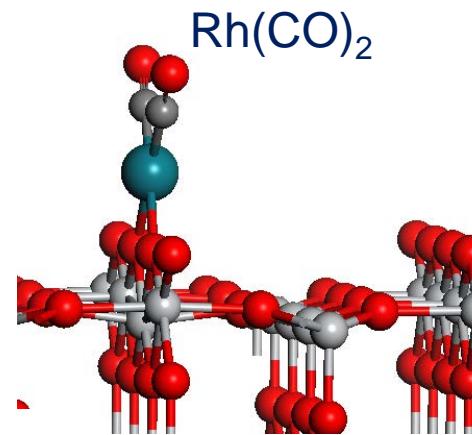
Formation energy = $E_{\text{adatom/support}} - E_{\text{support}} - E_{\text{bulk}}$

Using RPBE XC functional Slab model 6 layers thick

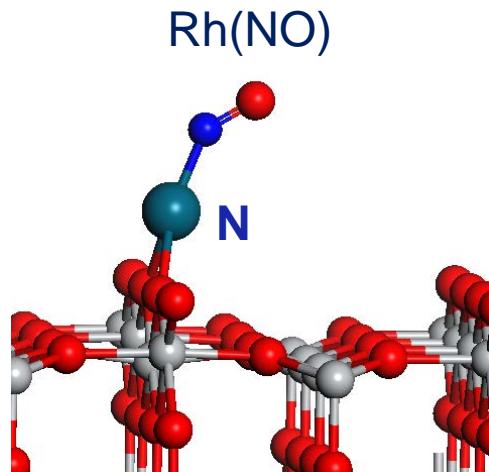
Rh(CO)₂ and Rh(NO)₂ have more favorable formation energies than Rh(CO) and Rh(NO)



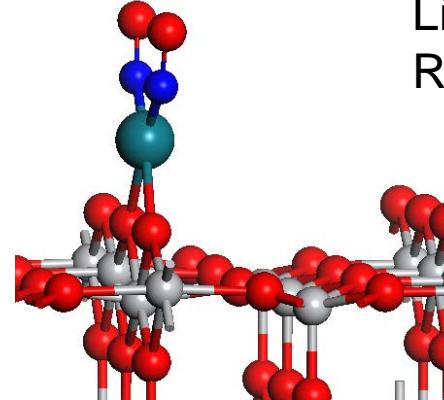
Formation energy = 0.75 eV



-1.35 eV



-0.02 eV



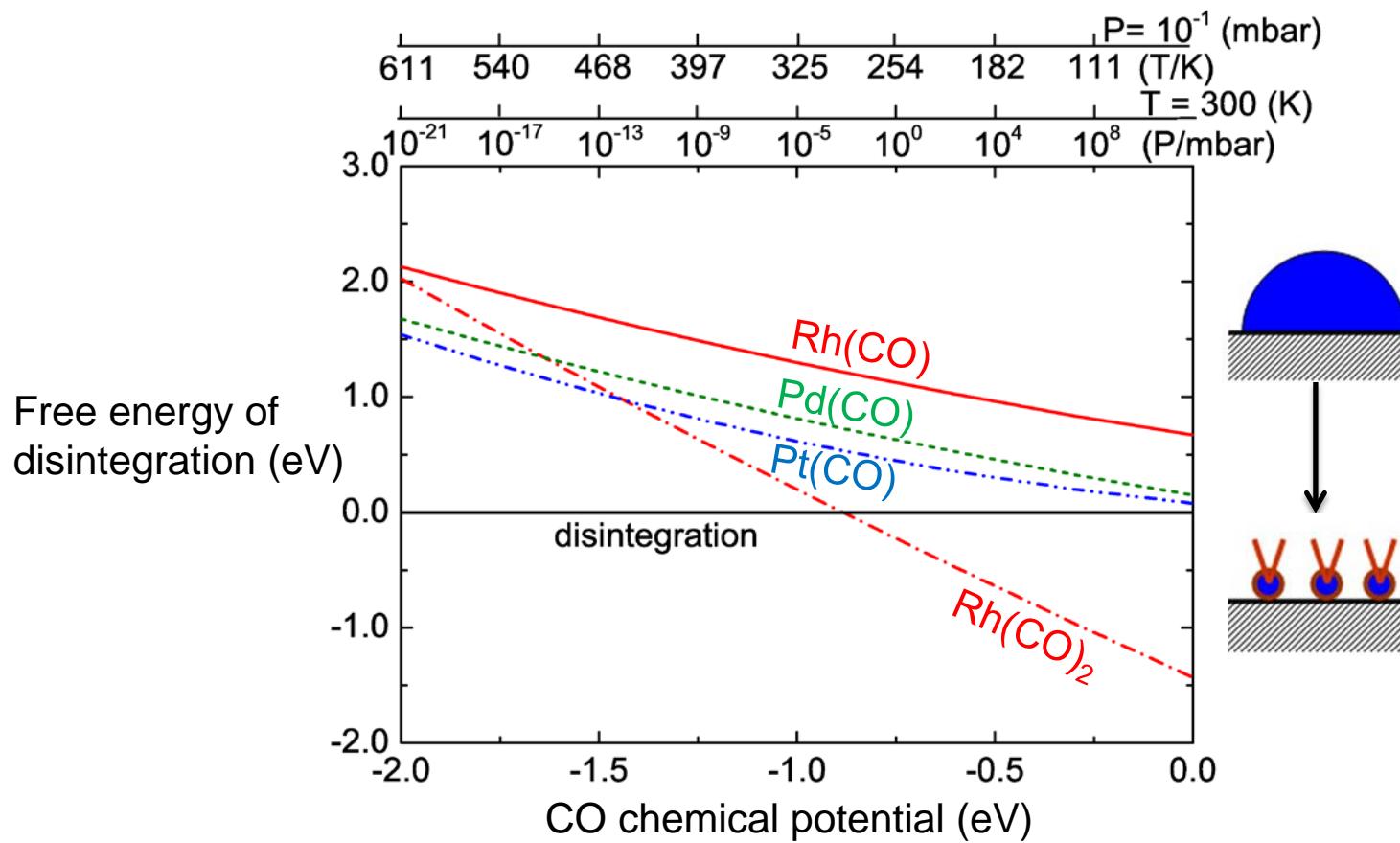
-1.58 eV

Literature evidence for stable
Rh(CO)₂ and Rh(NO)₂ [1-2]

[1] A. Suzuki *et al.*, *Angew. Chem. Int. Ed.* 42 (2003)

[2] A. Berkó, J. Szökő, F. Solymosi *Surf. Sci.* 566, (2004)

Predicting particle disintegration under CO environment



For a 2 nm particle on $TiO_2(110)$

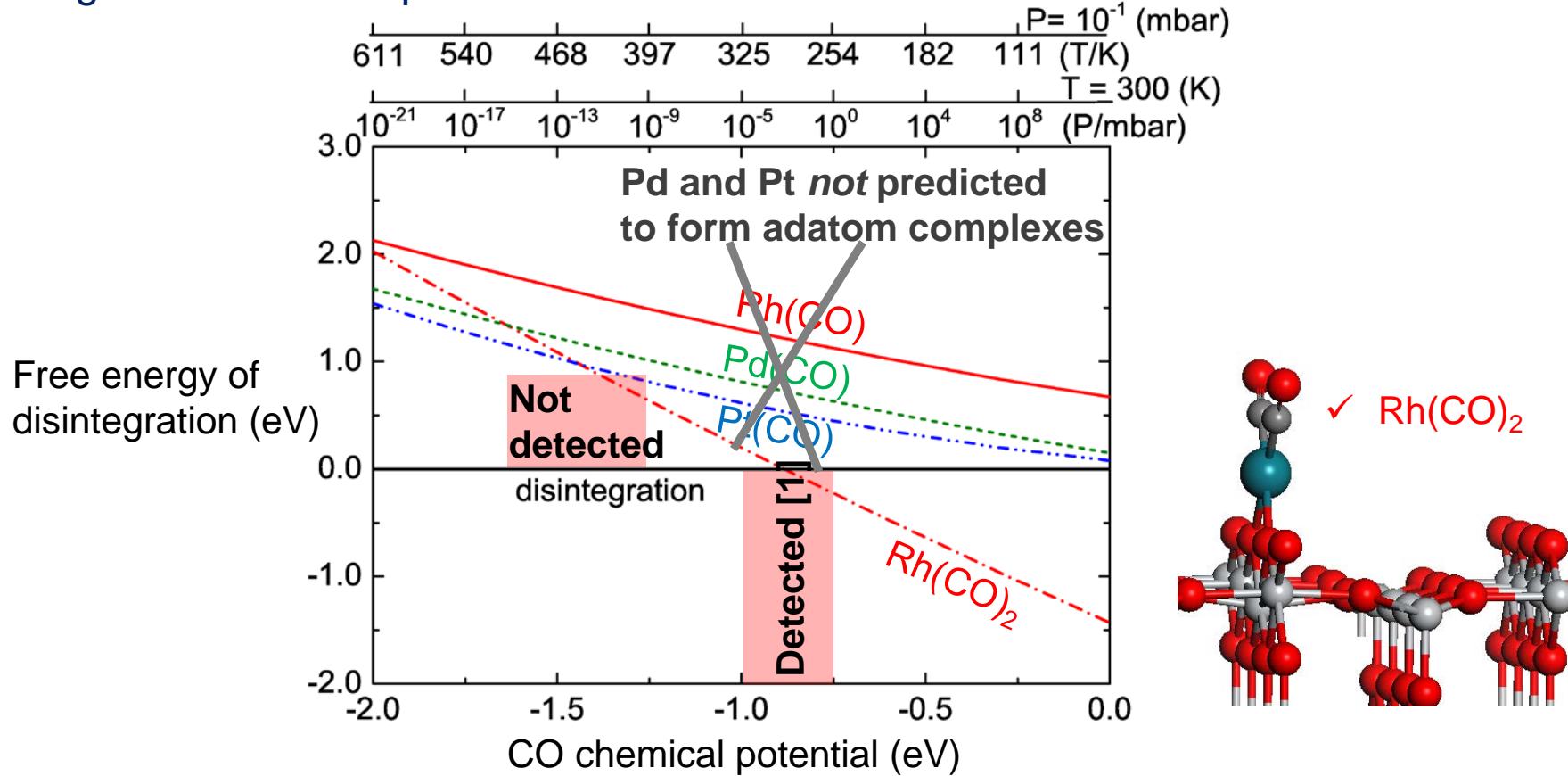
Only configurational entropy is included here, $\Theta = 0.01$ ML

[1] Berkó, A.; Szökő, J.; Solymosi, F. *Surf. Sci.* 566, 337 (2004)

[2] B. R. Goldsmith, E. D. Sanderson, R. Ouyang, W.-X. Li, *J. Phys. Chem. C* 118 (2014)

Rh(CO)₂ predicted to form stable complex
but not Rh(CO) at 300 K and 10⁻¹ mbar

In agreement with experimental observations



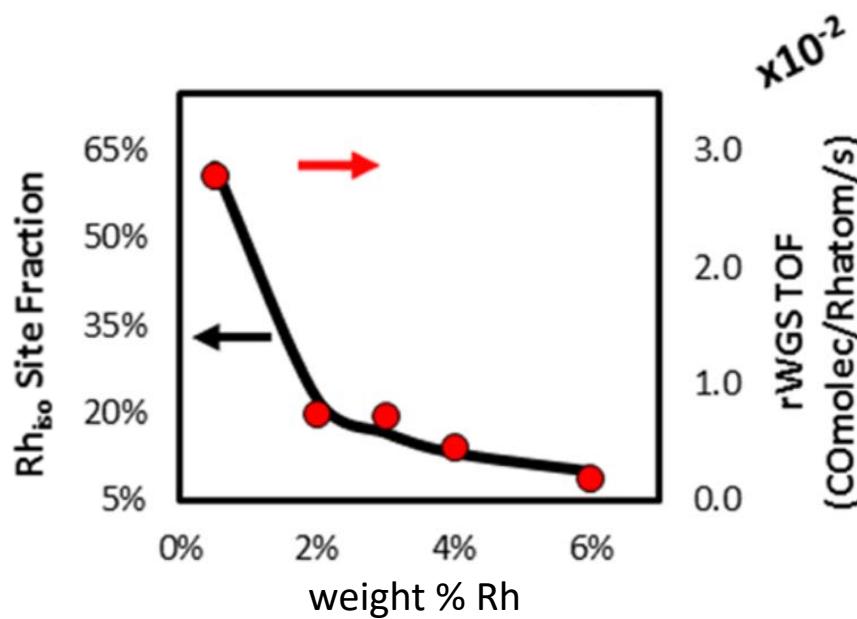
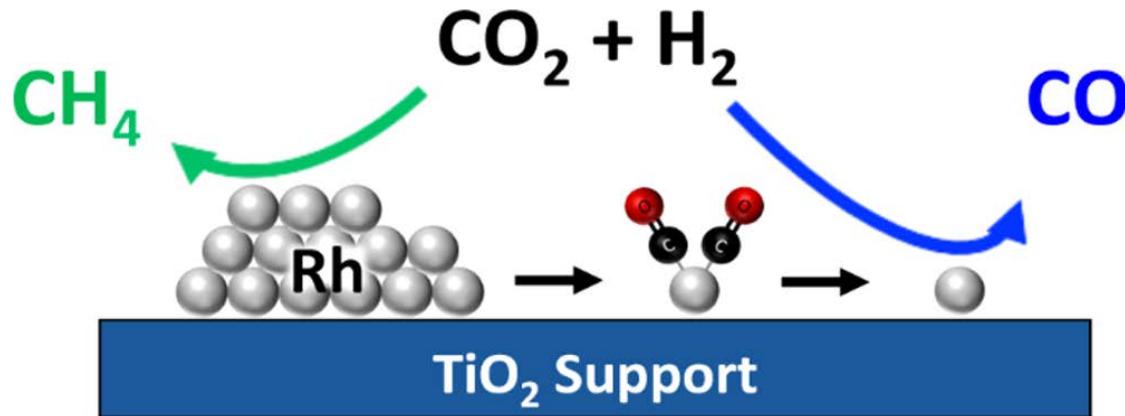
For a 2 nm particle on TiO₂(110)

Only configurational entropy is included here, $\Theta = 0.01$ ML

[1] Berkó, A.; Szökő, J.; Solymosi, F. *Surf. Sci.* 566, 337 (2004)

[2] B. R. Goldsmith, E. D. Sanderson, R. Ouyang, W.-X. Li, *J. Phys. Chem. C* 118 (2014)

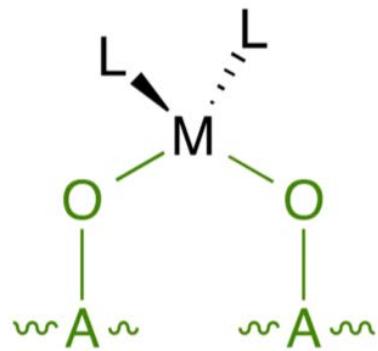
Isolated metal active site concentration and stability control catalytic CO₂ reduction selectivity



Modeling catalyst sites on amorphous supports has been a long-standing challenge

Lack of well-defined structure

Diversity of site environments

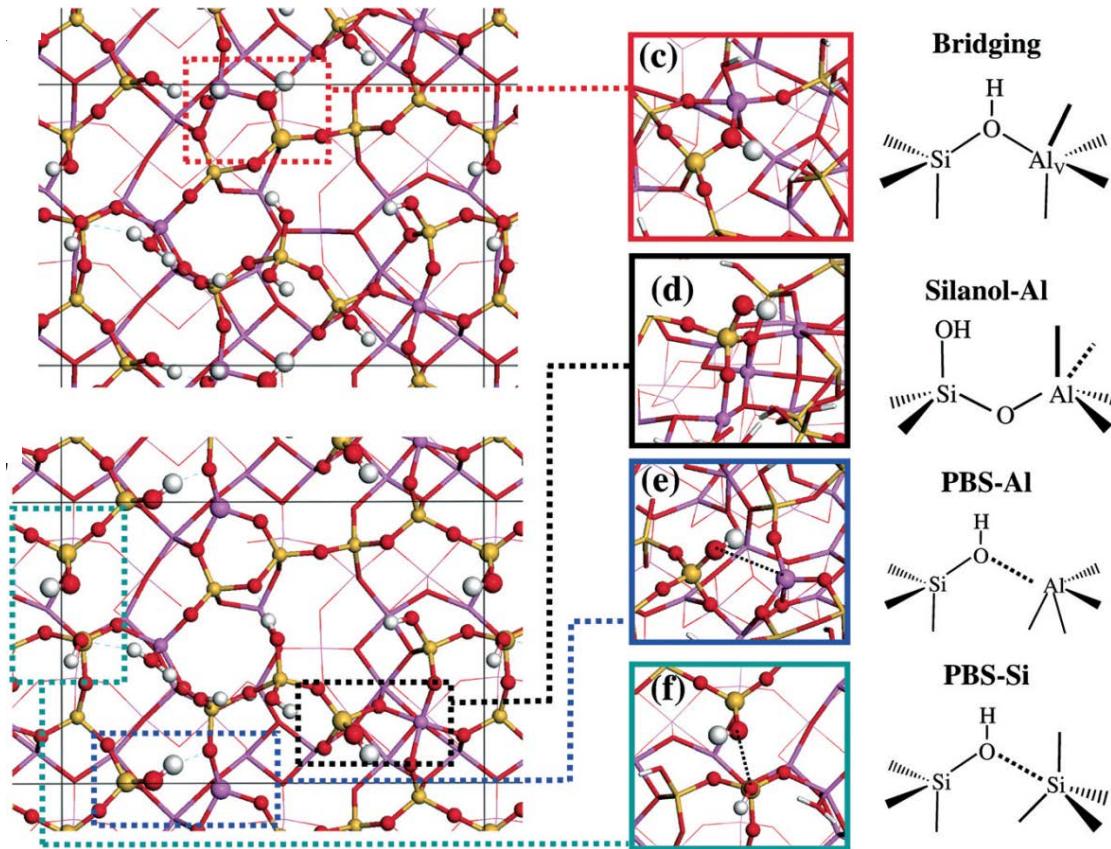


L = ligand

M = metal

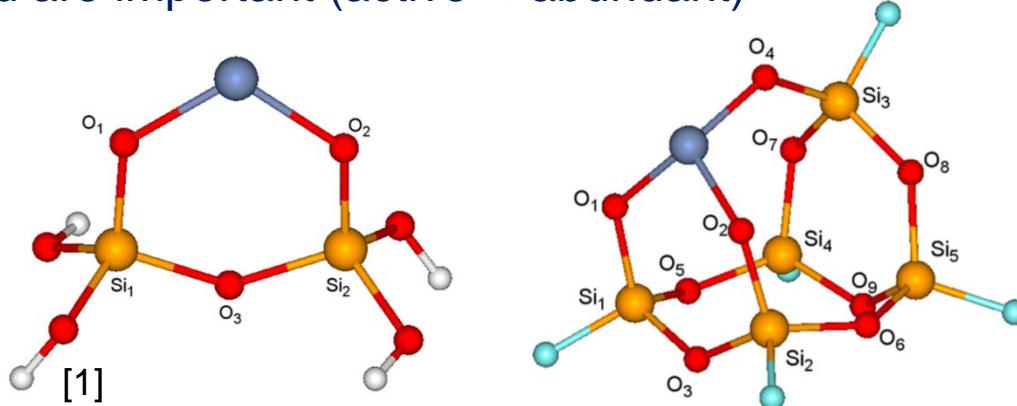
A = amorphous support

Example: Amorphous silica-alumina

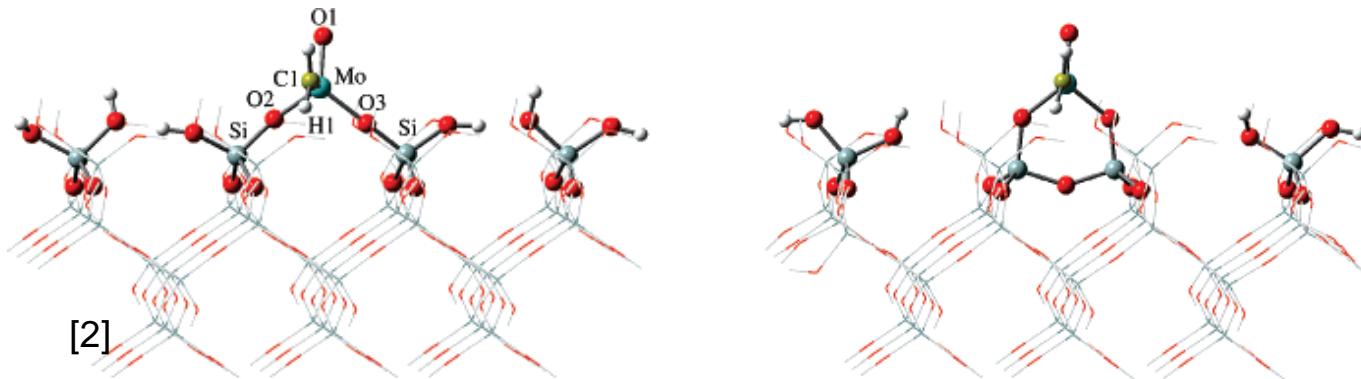


Typical modeling protocols for amorphous catalyst sites

Assume one or two cluster models capture main features and are important (active \times abundant)



Use a crystalline support with rigid constraints



- [1] A. Fong, Y. Yuan, S. Ivry, S. L. Scott, and B. Peters, *ACS Catal.* 5, 3360 (2015)
[2] J. Handzlik, *J. Phys. Chem.* 111, 26 (2007)

New approaches are needed to model amorphous catalysts

Sample the distribution of catalyst site environments

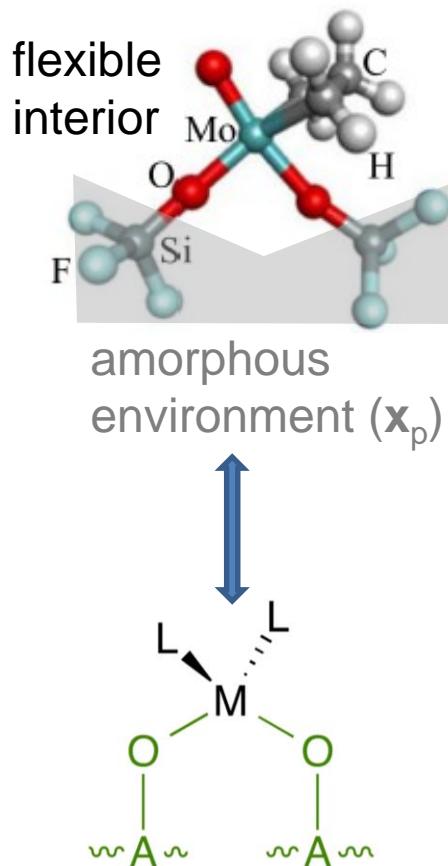
Identify the most important catalyst sites

Understand how local structural differences influence catalyst site reactivity

Systematically identify structure-reactivity relationships

New algorithms are needed
to sample the most important catalyst sites

Use only information we know



Our modeling premises

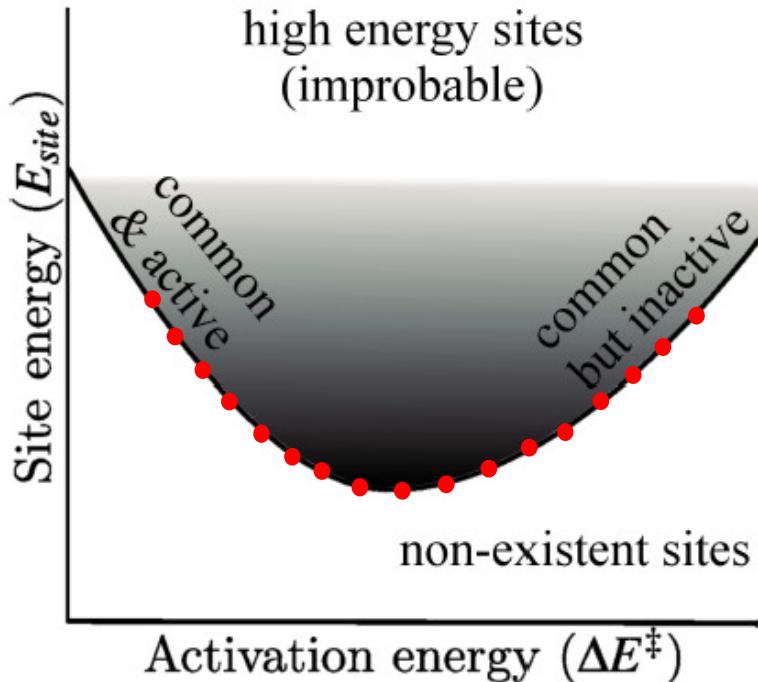
- 1) Periphery atoms (x_p) should be immobile
- 2) x_p influence chemical properties of the site
- 3) x_p arranged in an *unknown and continuous distribution*
- 4) For any $\Delta E^\ddagger(x_p)$, assume low energy sites prevalent

From properties to structures

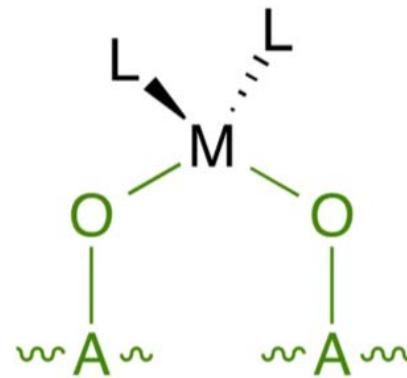
Use Sequential Quadratic Programming

$$\min_{\mathbf{x}_p} E_{red}^A(\mathbf{x}_p) \text{ subject to } \Delta E^\ddagger(\mathbf{x}_p) = \Delta E^\ddagger$$

Generate low energy catalyst structures with varying reactivity

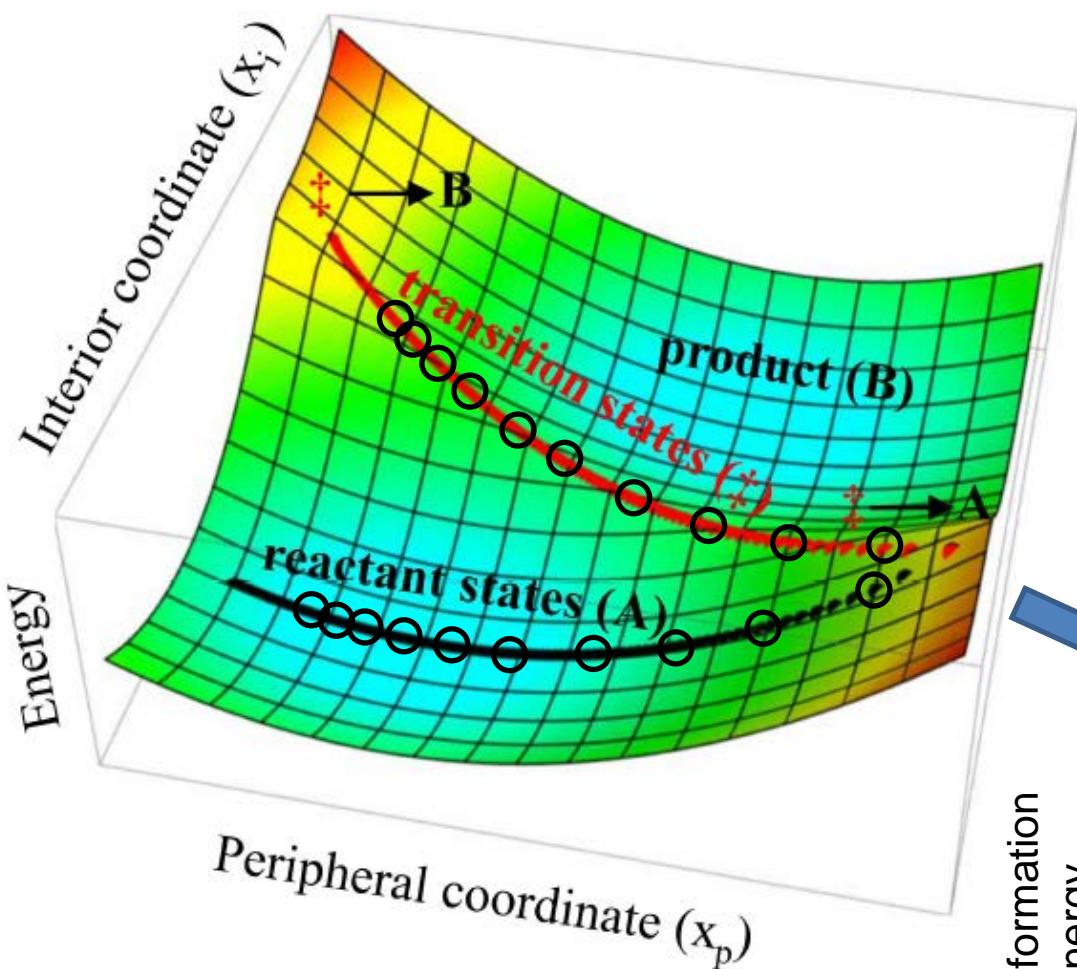


Each point on curve thought of as a different catalyst site



Different anchor point, $A = \mathbf{x}_p$

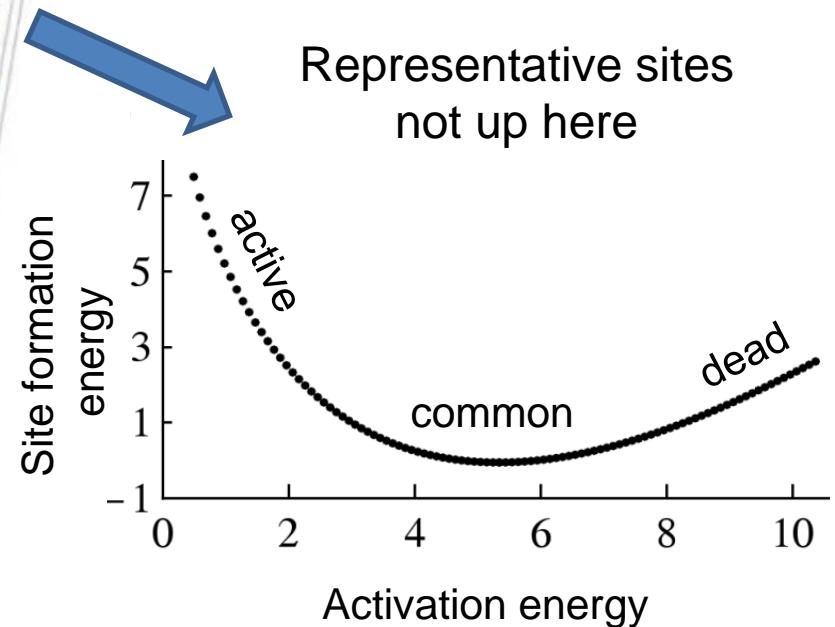
Example: Model Energy Landscape



$$\Delta \mathbf{x}_p = -(H_{red}^A)^{-1}(\mathbf{g}_{red}^A - \lambda \Delta \mathbf{g}_{red}).$$

$$\lambda = \frac{\Delta \Delta E^\ddagger + (\Delta \mathbf{g}_{red})^T (H_{red}^A)^{-1} \mathbf{g}_{red}^A}{(\Delta \mathbf{g}_{red})^T (H_{red}^A)^{-1} \Delta \mathbf{g}_{red}}.$$

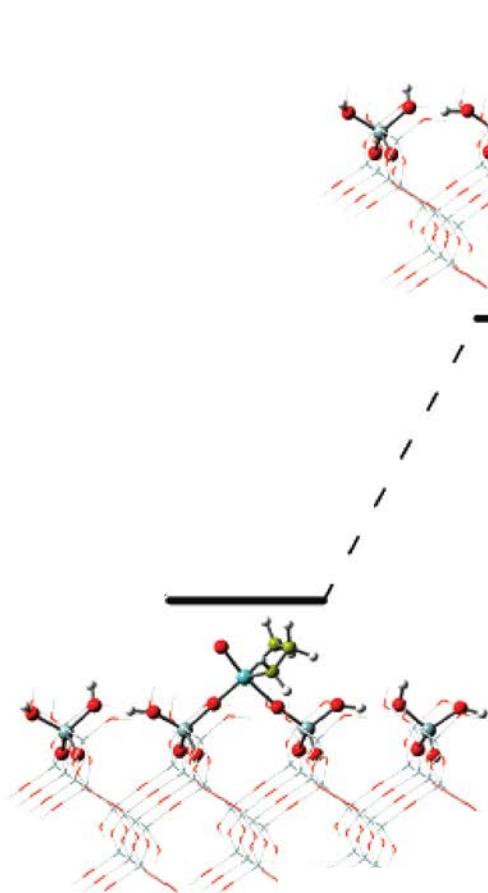
How do typical active and dead sites differ?



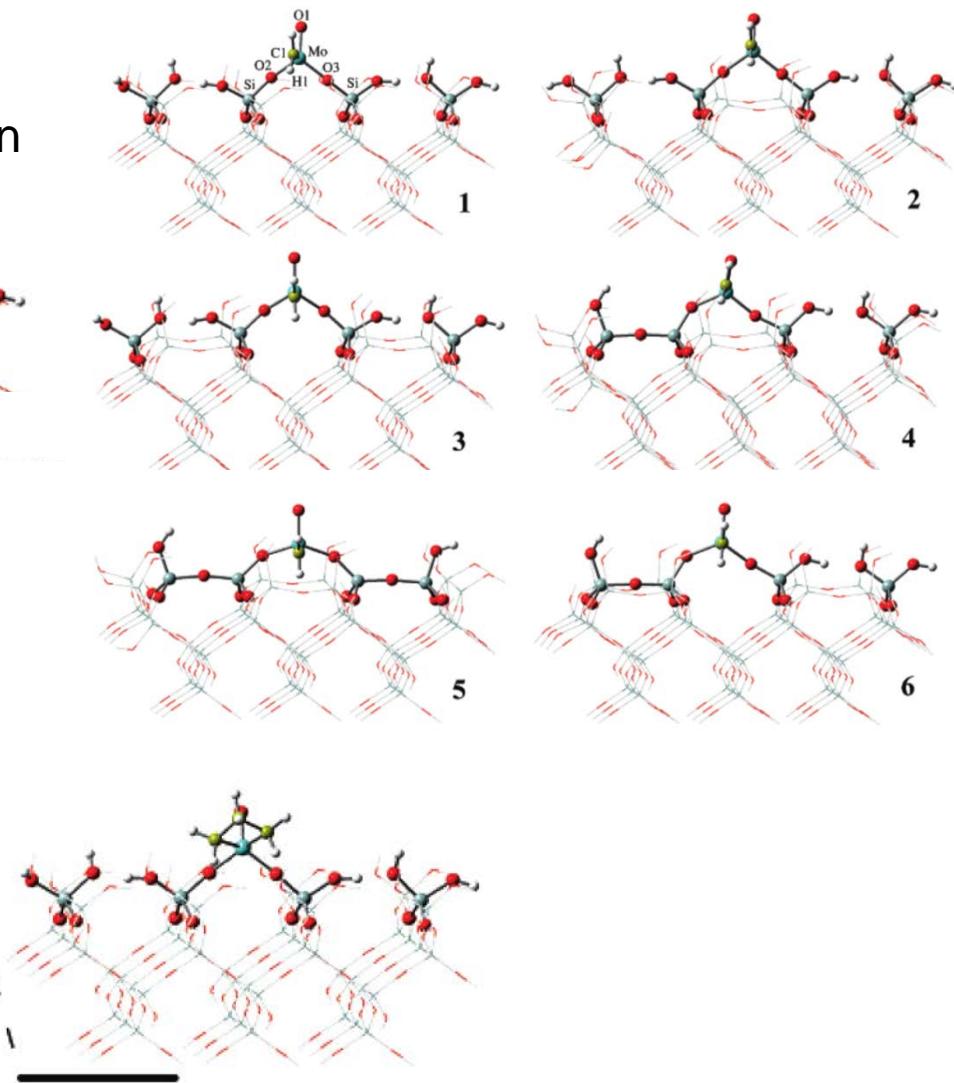
Ethene metathesis by isolated Mo(VI)/SiO₂

Handzlik used *ten* ONIOM
models from β -cristobalite

Metallacycle rotation

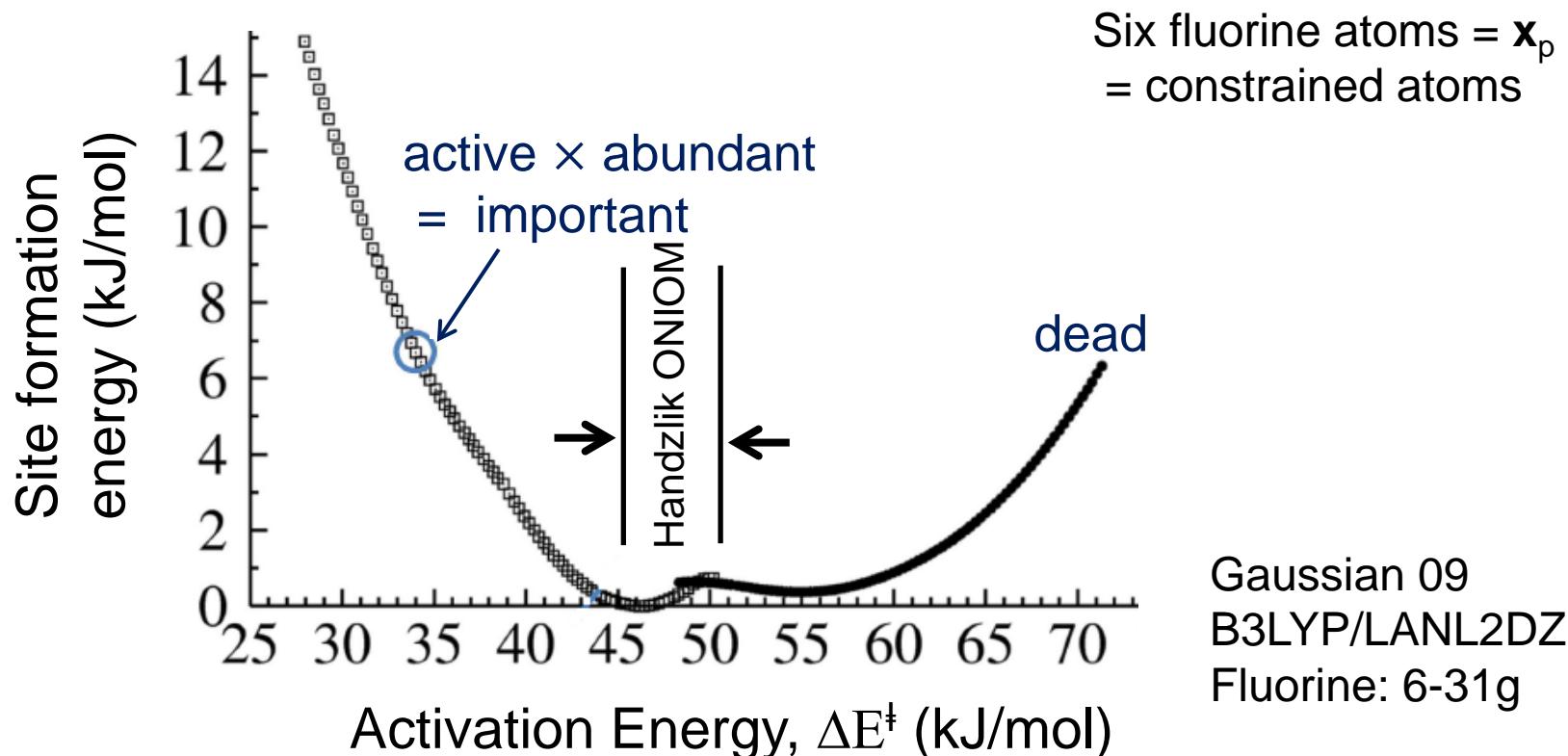
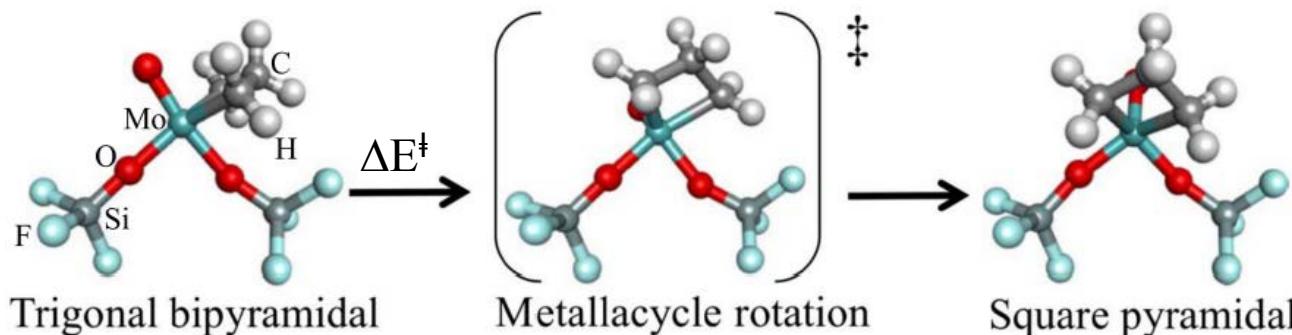


Trigonal bipyramidal



Square pyramidal

A large variance in activation energy is computed



[1] B. R. Goldsmith, E. D. Sanderson, D. Bean, B. Peters, *J. Chem. Phys.* 138, 204105 (2013)

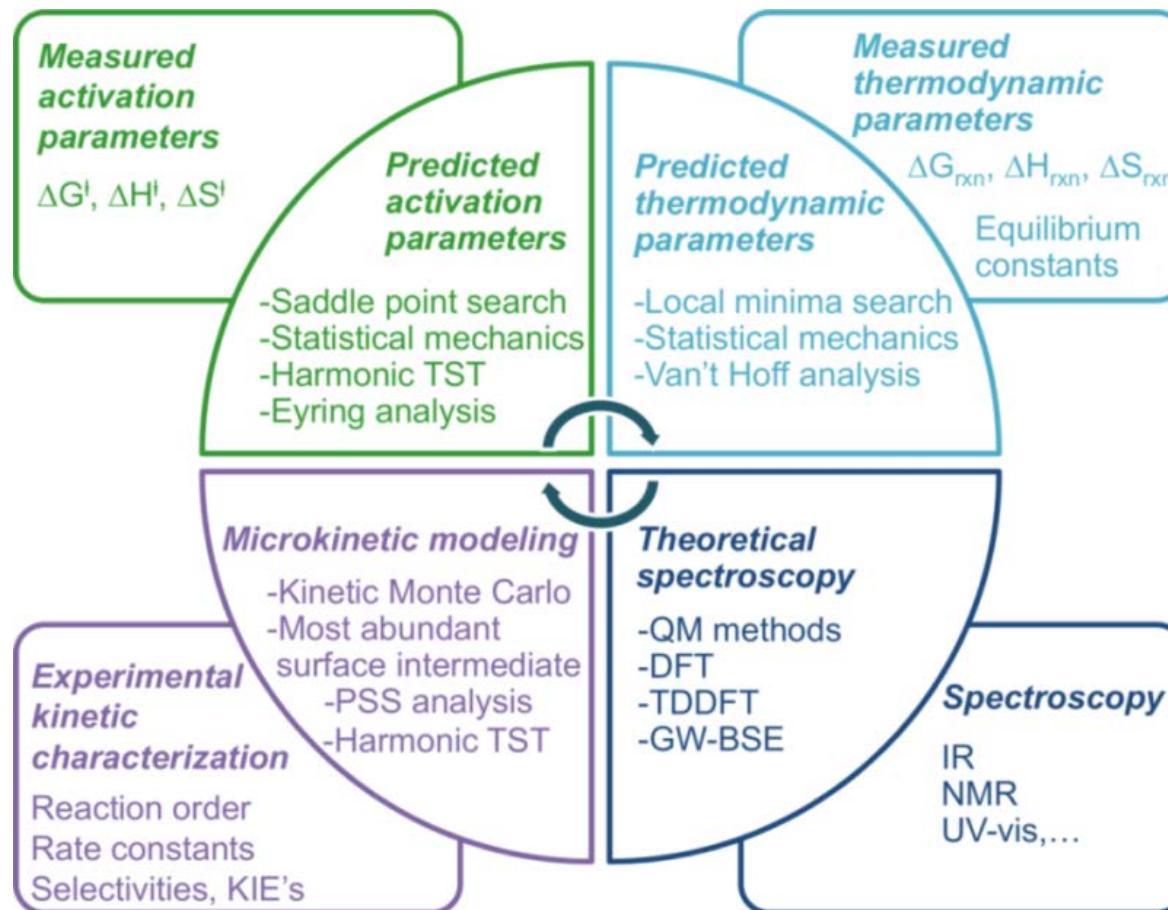
[2] B. R. Goldsmith *et al.* in *Reaction Rate Constant Computations: Theories and Applications*, RSC (2013)

Computational modeling is a powerful method for understanding catalysis at surfaces

Mechanistic hypothesis testing

Structure-property relationships

Catalyst screening and design



Acknowledgements

Thanks for your attention!
Any questions?

Prof. Karsten Reuter

Prof. Matthias Scheffler

Dr. Luca Ghiringhelli

Dr. Sergey Levchenko

Prof. Baron Peters

Prof. Susannah Scott



Alexander von Humboldt
Stiftung/Foundation

Fritz Haber Institute of the Max Planck Society
Theory Department

