Material Sciences and Solid-State Physics

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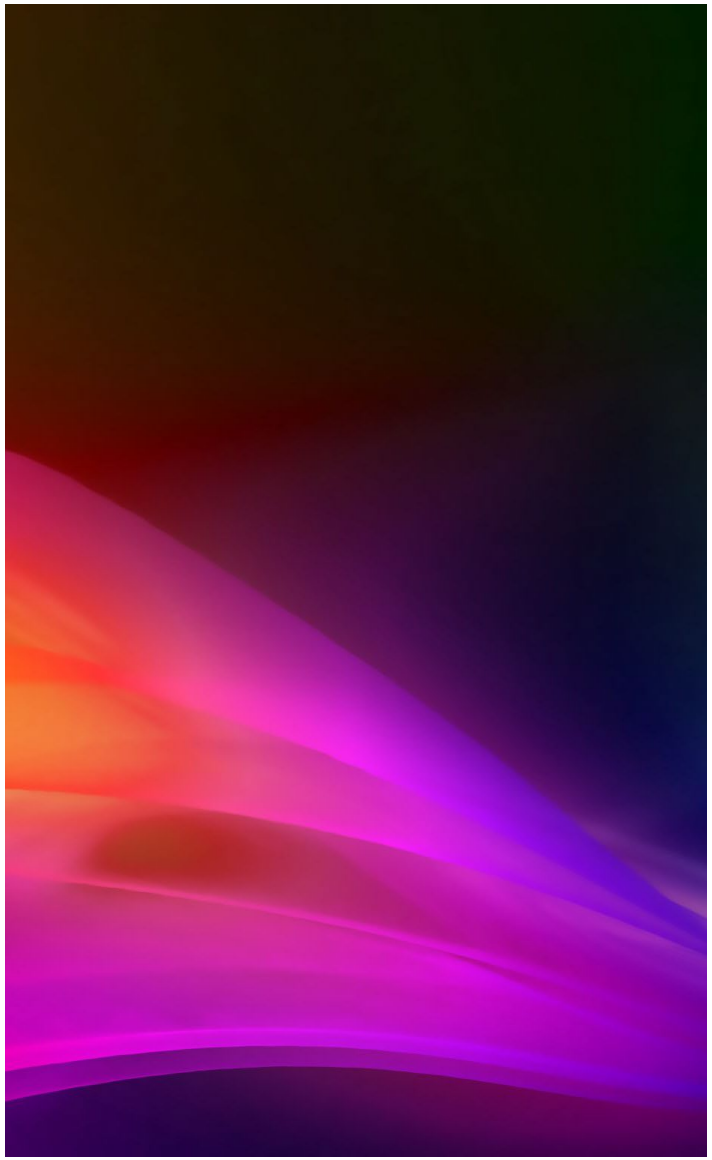
Transforming Computational Power into Environmental Solutions: HPC-driven Research on Urethanase-mediated Plastic Degradation

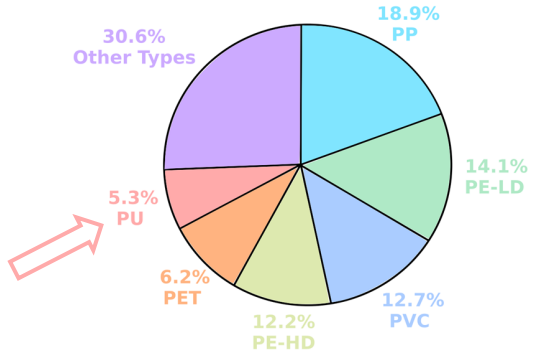


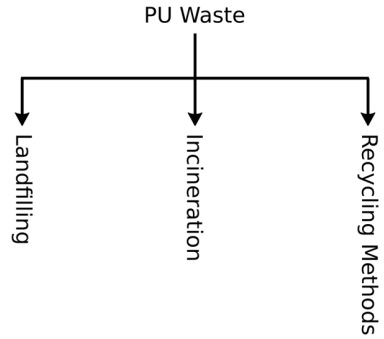
Luís M. C. Teixeira
PhD Candidate

Enzymatic Plastic Breakdown

Plastics > Versatile polymeric materials

Significant global accumulation





Enzymatic depolymerization

Enhancing the catalytic efficiency

Computational methods are essential for rational mutagenesis

- UMG-SP2
- UMG-SP3

Importance of HPC Access

Computational fields
- Capability
- Versatility

= Relevant for studying complex biological macromolecules

Protein Dynamics

Simulations

In-depth atomistic analysis

Statistically significant exploration of the conformational space

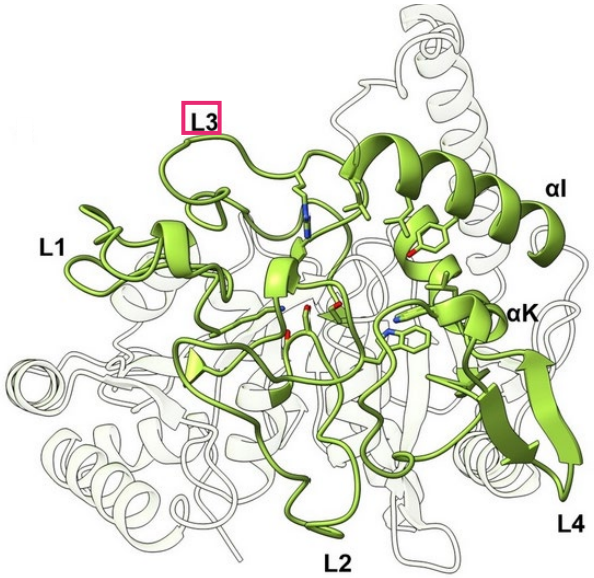
Enzyme Catalysis

Structural and energetic catalytic data

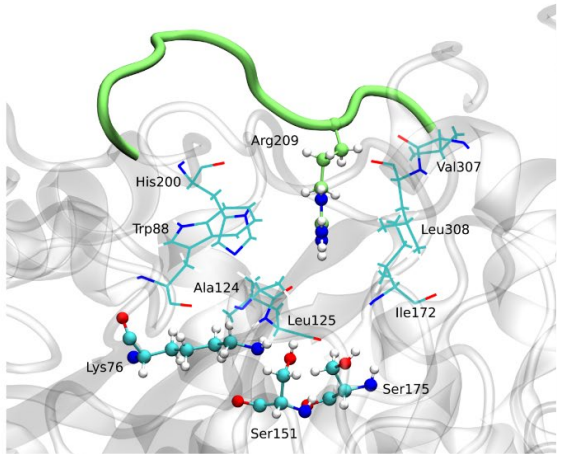
Hybrid QM/MM MD simulations (DFT)

Dynamical Behaviour – Substrate Recognition

HPC resources allowed us to simulate our systems throughout more than 50 us



Adapted from Angew. Chem. Int. Ed., 7, 2025



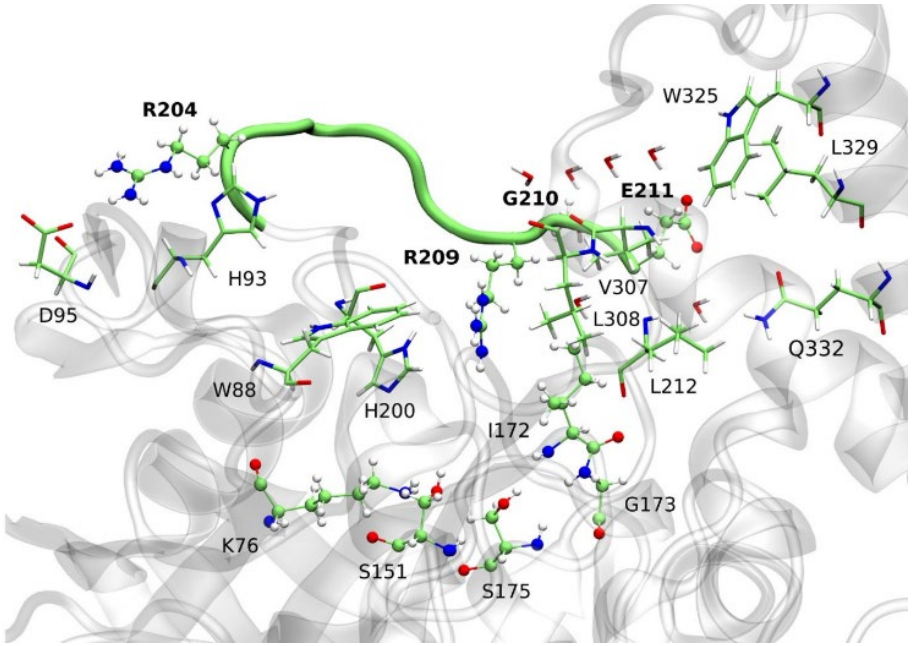
Our simulations confirmed the stability of both structural arrangements

Mutagenesis Study – Role of L3

L3 residues were targeted

- Computationally
- Experimentally

Simulations predicted productiveness



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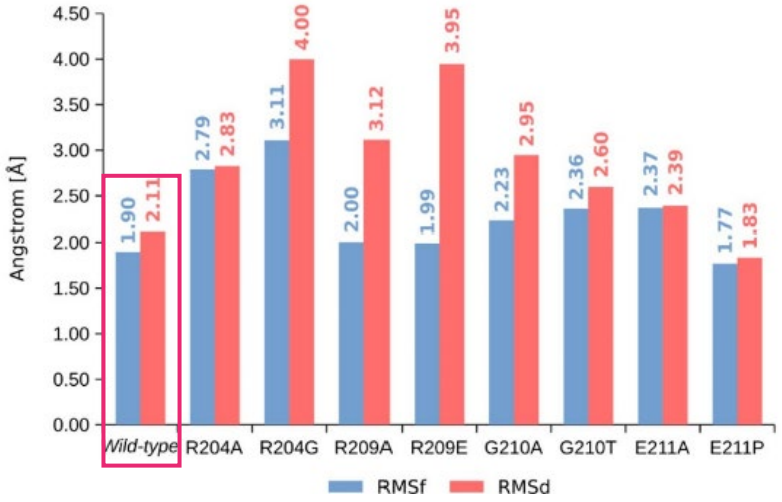
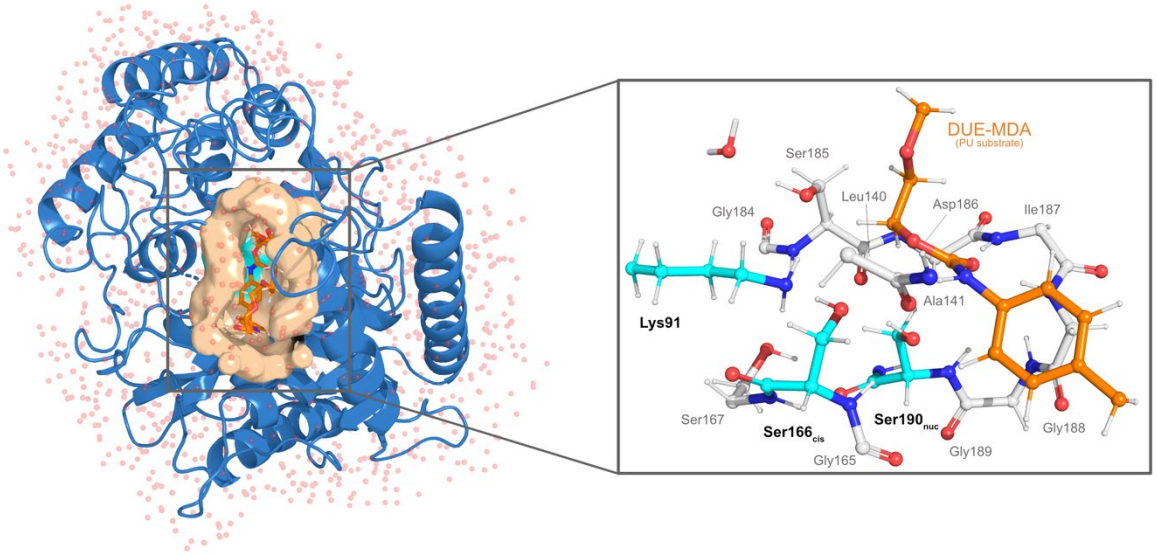


We speculated that a more mobile L3 would promote catalysis

Validation of Modelled Complex

Mechanistic study ⇨ Validated model

⚠ Lack of resolved complex structure



MD simulations confirmed the stability

- Protein fold
- Favourable Orientation

Constructed a QM/MM model to study the mechanism

UMG-SP2 Catalytic Mechanism

1) Catalytic triad facilitates proton shuttle
2) Ser_{nuc} conducts nucleophilic attack
3) A TI is formed and then collapsed
4) Ester bond cleavages releases an alcohol and yields AE
5) Bond cleavage is the rate-limiting step

1) Wat_{cat} occupies the vacant space
2) Wat_{cat} conducts the nucleophilic attack
3) AE is hydrolysed releasing
4) A highly unstable carbamic acid product is released
5) It is decomposed quickly into CO_2

Adapted from Chem. Sci., 16, 2025

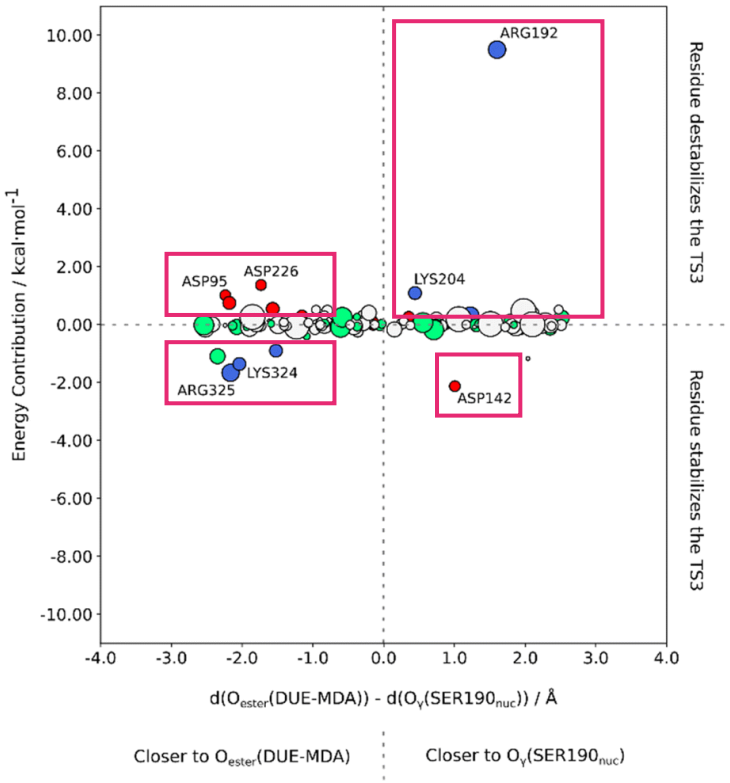
B3LYP/6-311+G(2d,2p)-D3(BJ): ff14SB//B3LYP/6-31G(d)-D3(BJ):ff14SB

Residue Energy Reassessment – Mutation Proposals

MM residues influence ⇨ 149 residues were systematically removed

⇩

Single-point energy calculations



No conformational rearrangement

⇩

Electrostatic influence roadmap

Elimination or replacement could reduce the energetic cost

✕

Improving catalytic efficiency

Adapted from Chem. Sci., 16, 2025

Conclusion

1) Computational approaches were fundamental for understanding conformational dynamics and the catalytic mechanism of UMG-SP2 and UMG-SP3
2) EuroHPC resources were a cornerstone of this work (large simulation timescales and QM-MM resolution of the free energy profile)
3) Relevant role of HPC-driven work in advancing protein research
4) Synergy between large-scale computational resources and enzymatic knowledge enhance our understanding of plastic biodegradation

Unveiling the enzymatic pathway of UMG-SP2 urethanase: insights into polyurethane degradation at the atomic level†

P. Paiva [ab], L. M. C. Teixeira [ab], R. Wei [c], W. Liu [d], G. Weber [e], J. P. Morth [bf], P. Westh [bf], A. R. Petersen [bg], M. B. Johansen [bg], A. Sommerfeldt [bg], A. Sandahl [bg], D. E. Otzen [bh], P. A. Fernandes [ab] and M. J. Ramos [*ab]

Chemical Science, doi:10.1039/d4sc06688j

Structural and Functional Characterization of an Amidase Targeting a Polyurethane for Sustainable Recycling

Laura Rotilio, Thomas Bayer, Hannes Meinert, Luis M. C. Teixeira, Martin B. Johansen, Andreas Sommerfeldt, Allan R. Petersen, Alexander Sandahl, Malene B. Keller, Jesper Holck, Pedro Paiva, Daniel E. Otzen, Uwe T. Bornscheuer, Ren Wei, Pedro A. Fernandes, Maria J. Ramos, Peter Westh, and J. Preben Morth**

Angewandte Chemie International Edition, doi:10.1002/anie.202419535

Structure-Guided Engineering of a Versatile Urethanase Improves Its Polyurethane Depolymerization Activity

Zhishuai Li, Xu Han, Lin Cong, Parinita Singh, Pedro Paiva, Yannick Branson, Wenshuo Li, Yangyang Chen, Da'san M. M. Jaradat, Frank Lennartz, Thomas Bayer, Louis Schmidt, Ulrike Garscha, Song You, Pedro Alexandrino Fernandes, Maria João Ramos, Uwe T. Bornscheuer, Gert Weber, Ren Wei,* and Weidong Liu**

Advanced Science, doi:10.1002/advs.202416019

Acknowledgments

HPC in Molecular Modeling Group

En'Zync Consortium

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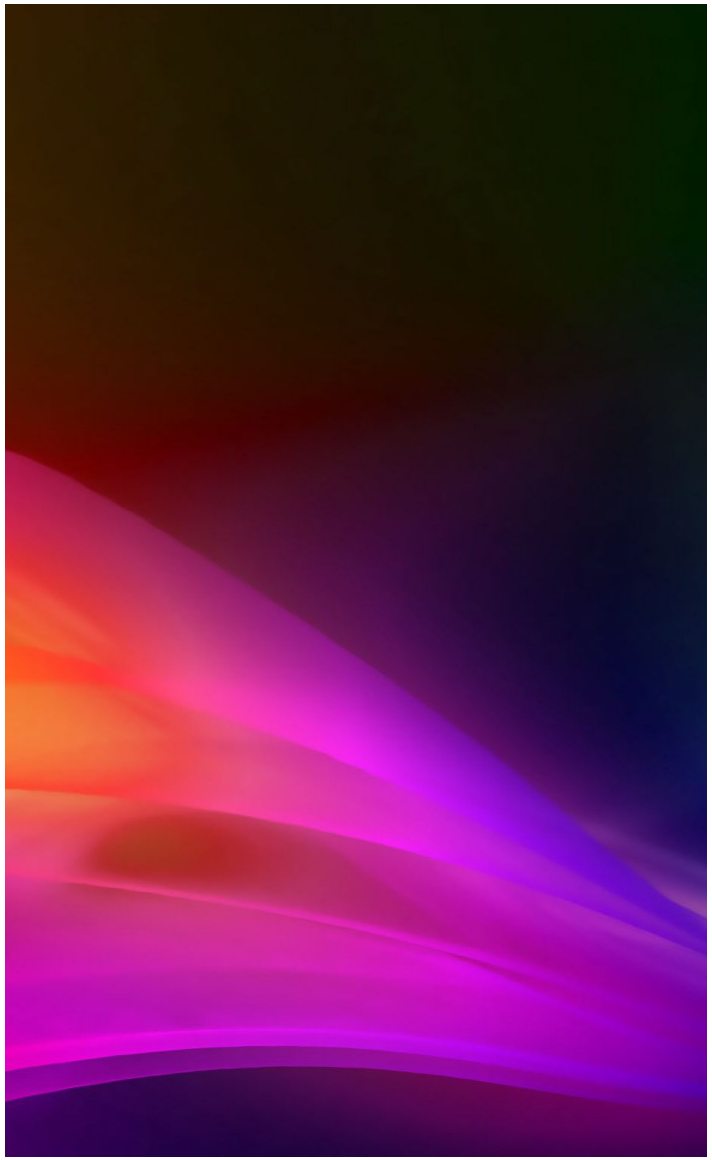
Transforming Computational Power into Environmental Solutions: HPC-driven Research on Urethanase-mediated Plastic Degradation



Luís M. C. Teixeira
PhD Candidate

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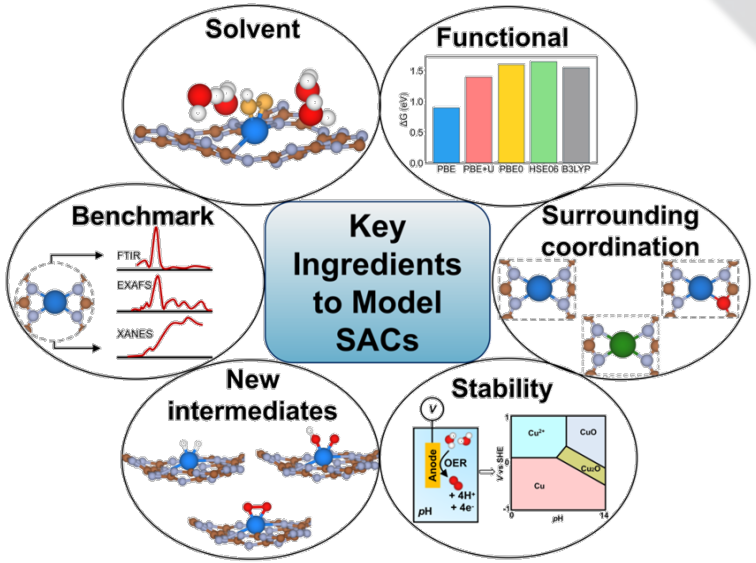
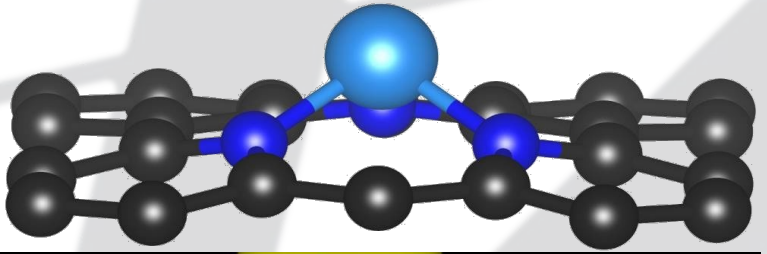
Coordination Chemistry on Single-Atom Alloys



Giovanni Di Liberto
giovanni.diliberto@unimib.it



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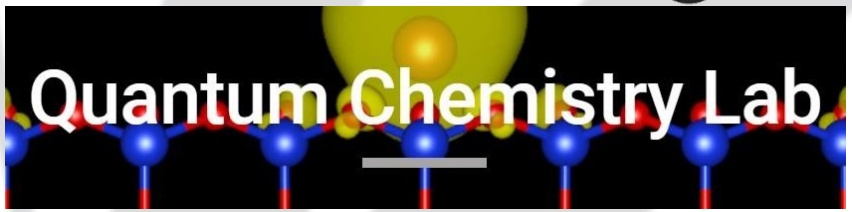
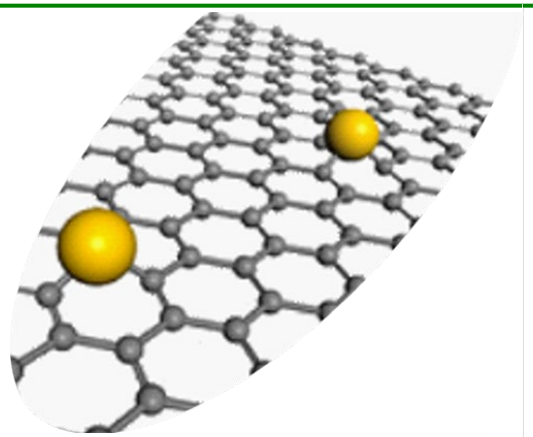
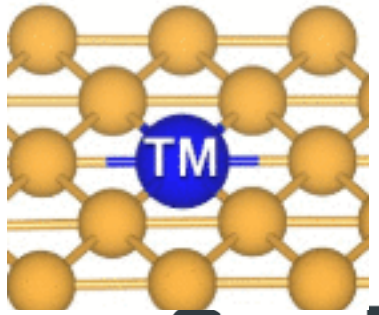
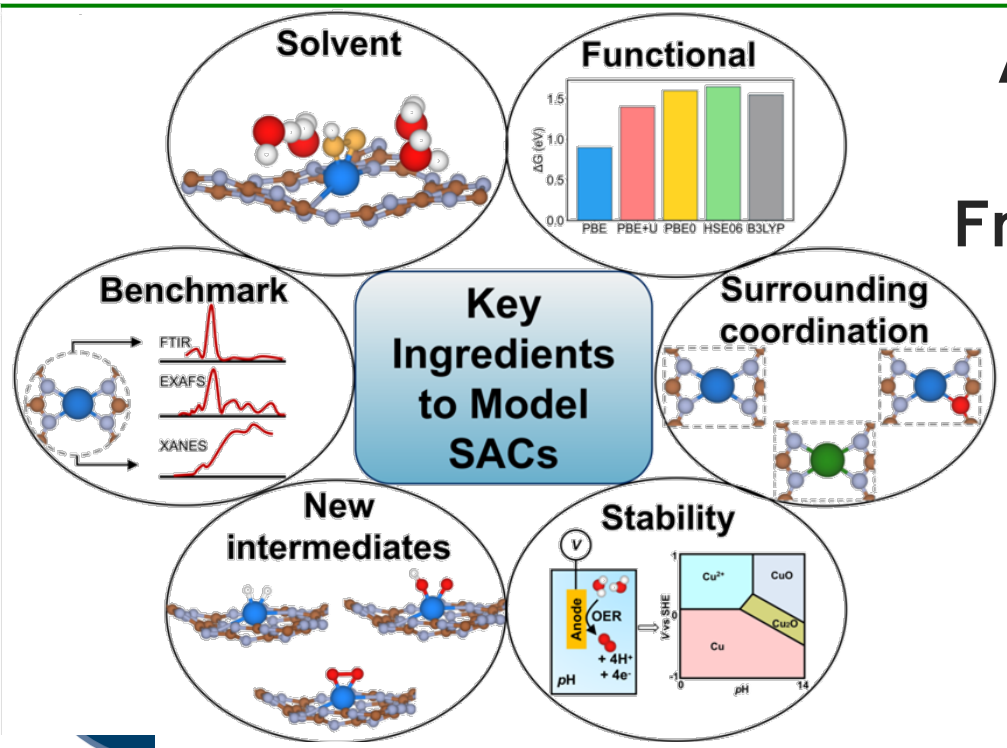
30th September 2025



Outline







Application of Quantum Chemical Simulations

From Computational Framework to Applications

Chem Soc Rev
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Interfacing single-atom catalysis with continuous-flow organic electrosynthesis

Mark A. Bajada, Jesús Sanjosé-Orduna, Giovanni Di Liberto, Sergio Tosoni, Gianfranco Pacchioni, Timothy Noël and Gianvito Vilé

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Article

An Adaptive Palladium Single-Atom Catalyst Enabling Reactivity Switching between Borylation and C–C Coupling

Vitthal B. Saptal, Clara Saetta, Adriana Laufenböck, Martin Sterrer, Ik Seon Kwon, Andrea Lucotti, Matteo Tommasini, Ondřej Tomanec, Aristides Bakandritsos, Giovanni Di Liberto,* Gianfranco Pacchioni, and Gianvito Vilé*

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Research Article

Tracking Charge Dynamics in a Silver Single-Atom Catalyst During the Light-Driven Oxidation of Benzyl Alcohol to Benzaldehyde

Areti Moutsiou, Andrea Olivati, Luis A. Cipriano, Alessandra Sivo, Sean M. Collins, Quentin M. Ramasse, Ik Seon Kwon, Giovanni Di Liberto, Mohamad Kanso, Robert Wojcieszak, Gianfranco Pacchioni, Annamaria Petrozza, and Gianvito Vilé*

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Research Article

Azide-Alkyne Click Chemistry over a Heterogeneous Copper-Based Single-Atom Catalyst

Gianvito Vilé,* Giovanni Di Liberto, Sergio Tosoni, Alessandra Sivo, Vincenzo Ruta, Maarten Nachtegaal, Adam H. Clark, Stefano Agnoli, Yajun Zou, Aleksandr Savateev, Markus Antonietti, and Gianfranco Pacchioni

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The Modelling Approach is Taken From Heterogenous Catalysis

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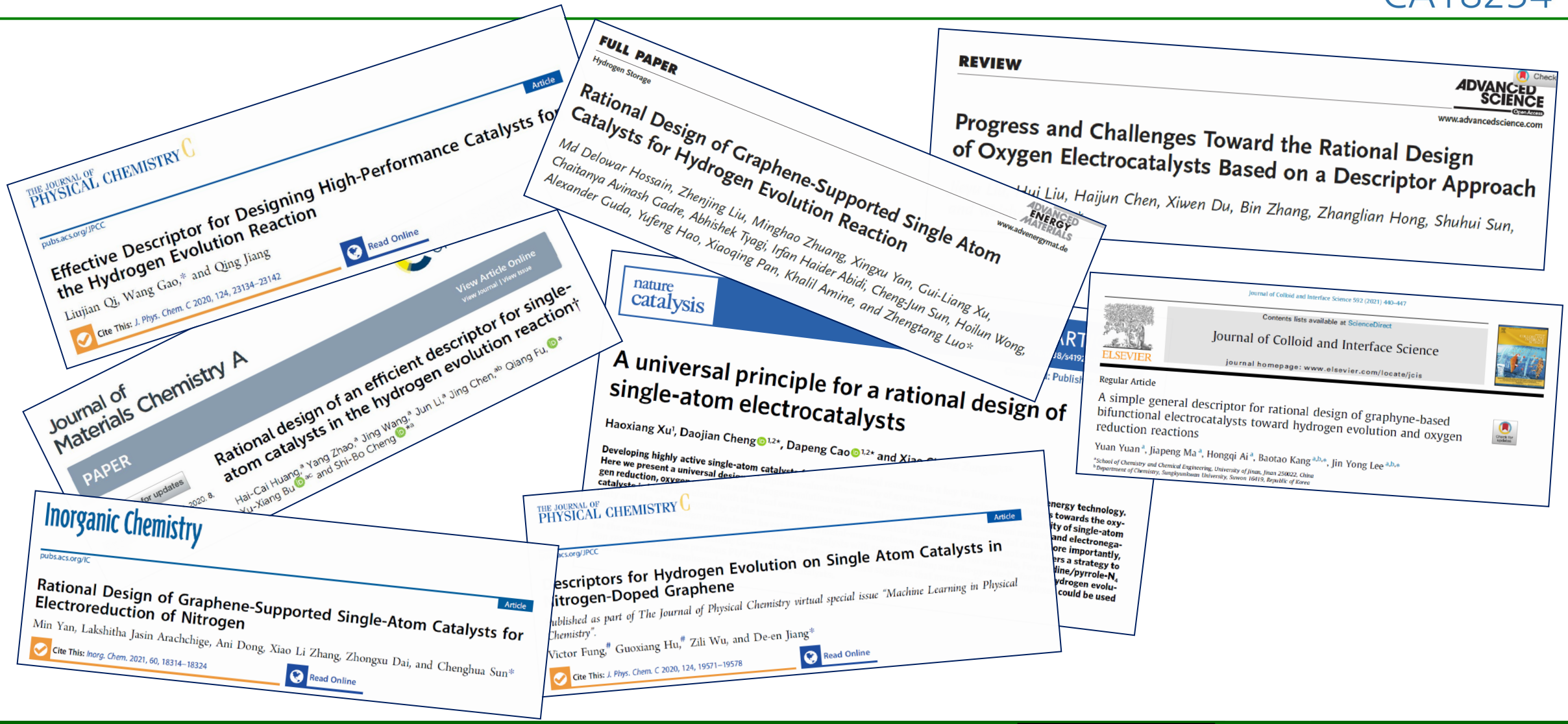

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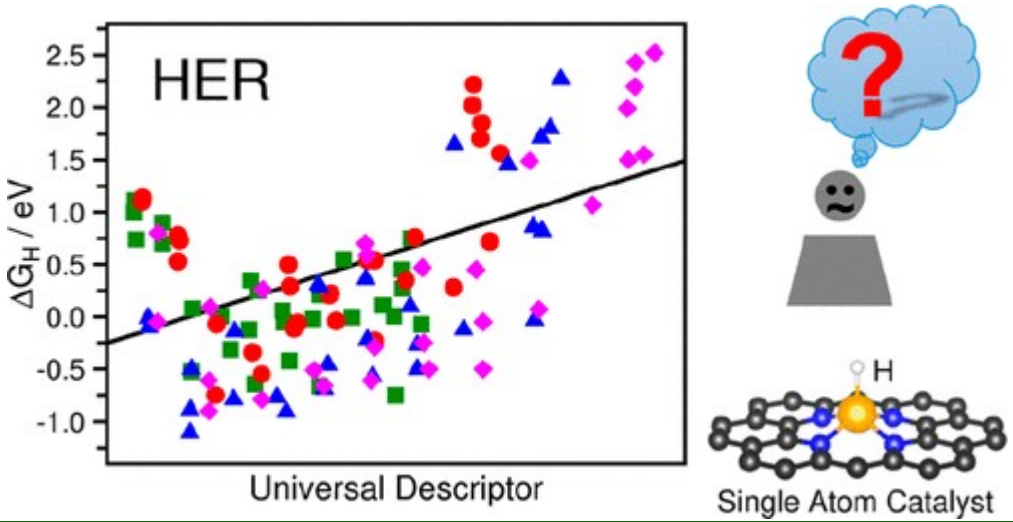
Universal Principles for the Rational Design of Single Atom Electrocatalysts? Handle with Care

Giovanni Di Liberto, Luis A. Cipriano, and Gianfranco Pacchioni*



nature catalysis

A universal principle for a rational design of single-atom electrocatalysts

ARTICLES

https://doi.org/10.1038/s41929-018-0063-z

Corrected: Publisher Corr

RETRACTED ARTICLE: A universal principle for a rational design of single-atom electrocatalysts

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Proposed Approach

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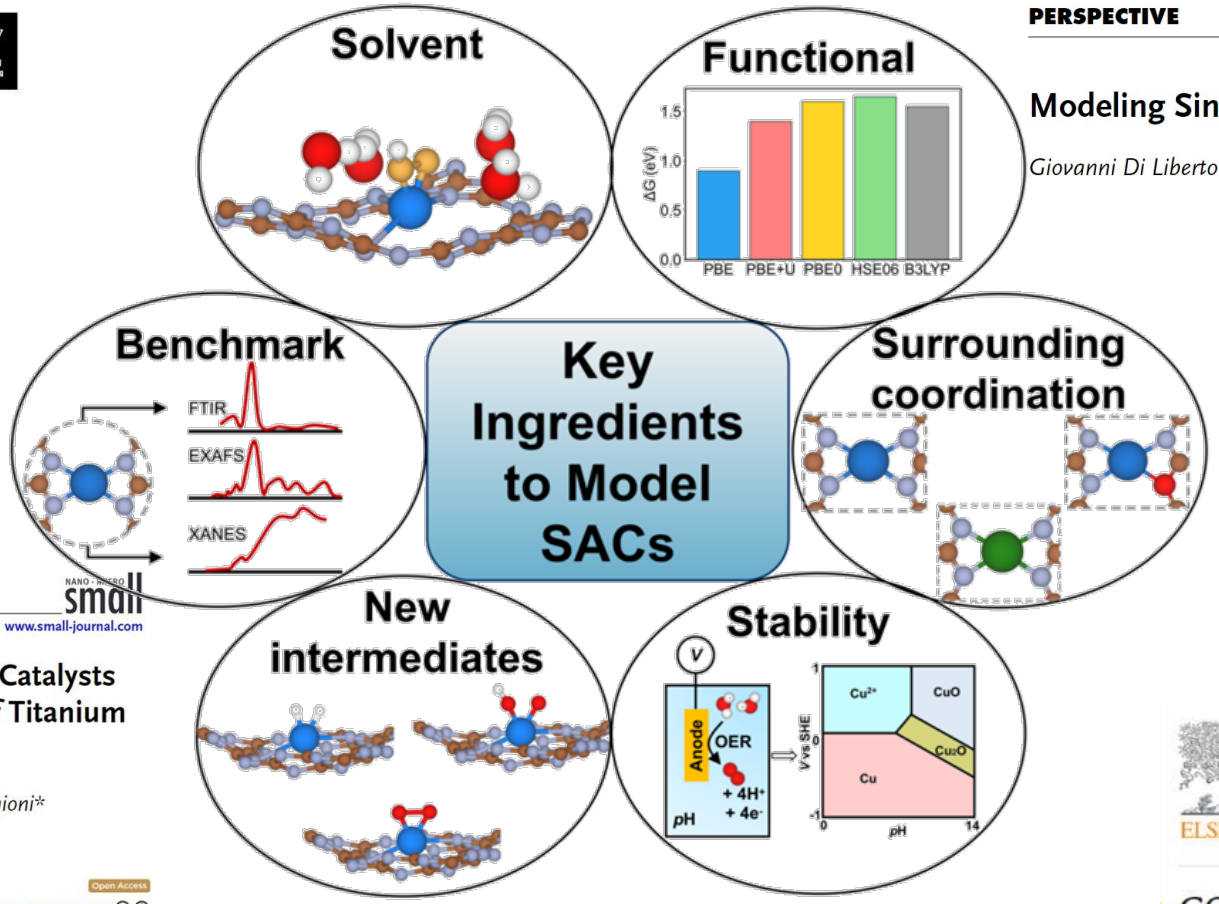

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Single Atom Catalysts: What Matters Most, the Active Site or The Surrounding?

Giovanni Di Liberto, Luis A. Cipriano, Prof. Dr. Gianfranco Pacchioni

ADVANCED THEORY AND SIMULATIONS

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Modeling Hydrogen and Oxygen Evolution Reactions on Single Atom Catalysts with Density Functional Theory: Role of the Functional

Ilaria Barlocco, Luis A. Cipriano, Giovanni Di Liberto, Gianfranco Pacchioni

RESEARCH ARTICLE

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Key Ingredients for the Screening of Single Atom Catalysts for the Hydrogen Evolution Reaction: The Case of Titanium Nitride

Clara Saetta, Ilaria Barlocco, Giovanni Di Liberto, and Gianfranco Pacchioni**

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Predicting the Stability of Single-Atom Catalysts in Electrochemical Reactions

Giovanni Di Liberto, Livia Giordano,* and Gianfranco Pacchioni*

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Modeling Single-Atom Catalysis

*Giovanni Di Liberto and Gianfranco Pacchioni**

ELSEVIER
Journal of Catalysis
Volume 417, January 2023, Pages 351-359

Does the Oxygen Evolution Reaction follow the classical OH*, O*, OOH* path on single atom catalysts?

Ilaria Barlocco, Luis A. Cipriano, Giovanni Di Liberto, Gianfranco Pacchioni

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Superoxo and Peroxo Complexes on Single-Atom Catalysts: Impact on the Oxygen Evolution Reaction

Luis A. Cipriano, Giovanni Di Liberto,* and Gianfranco Pacchioni

ELSEVIER
Journal of Catalysis
Volume 422, June 2023, Pages 1-11

CO_2 electroreduction on single atom catalysts: Is water just a solvent?

Debolina Misra [a,b], Giovanni Di Liberto [b], Gianfranco Pacchioni [b]

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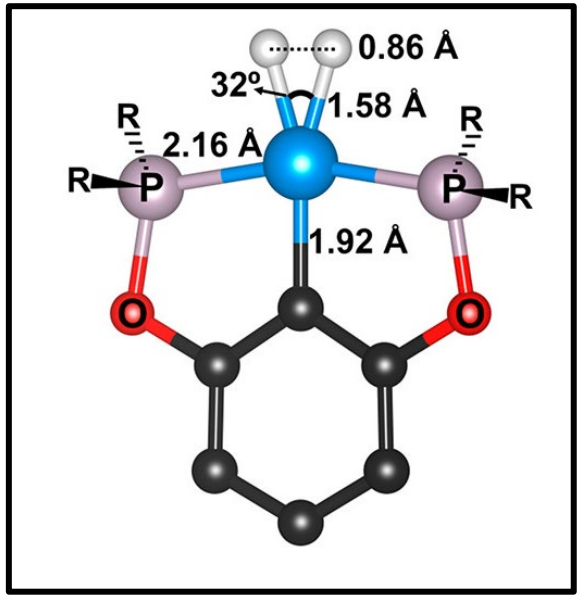
Reshaping the Modelling Approach



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VIP Cobalt Complexes

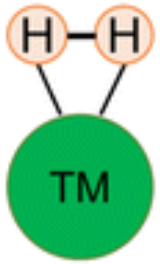
Preparation of a Dihydrogen Complex of Cobalt

Luis A. Cipriano

$d_{H\text{-}H} \approx 0.75$ Å

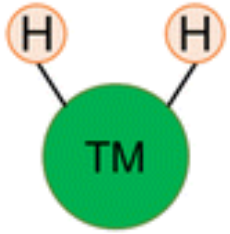
H_2^{phys}

0.77 Å > $d_{H\text{-}H}$ > 1.50 Å



H_2*

$d_{H\text{-}H}$ > 1.50 Å



H*H*

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Article

Role of Dihydride and Dihydrogen Complexes in Hydrogen Evolution Reaction on Single-Atom Catalysts

Giovanni Di Liberto,[#] Luis A. Cipriano, and Gianfranco Pacchioni*,[#]

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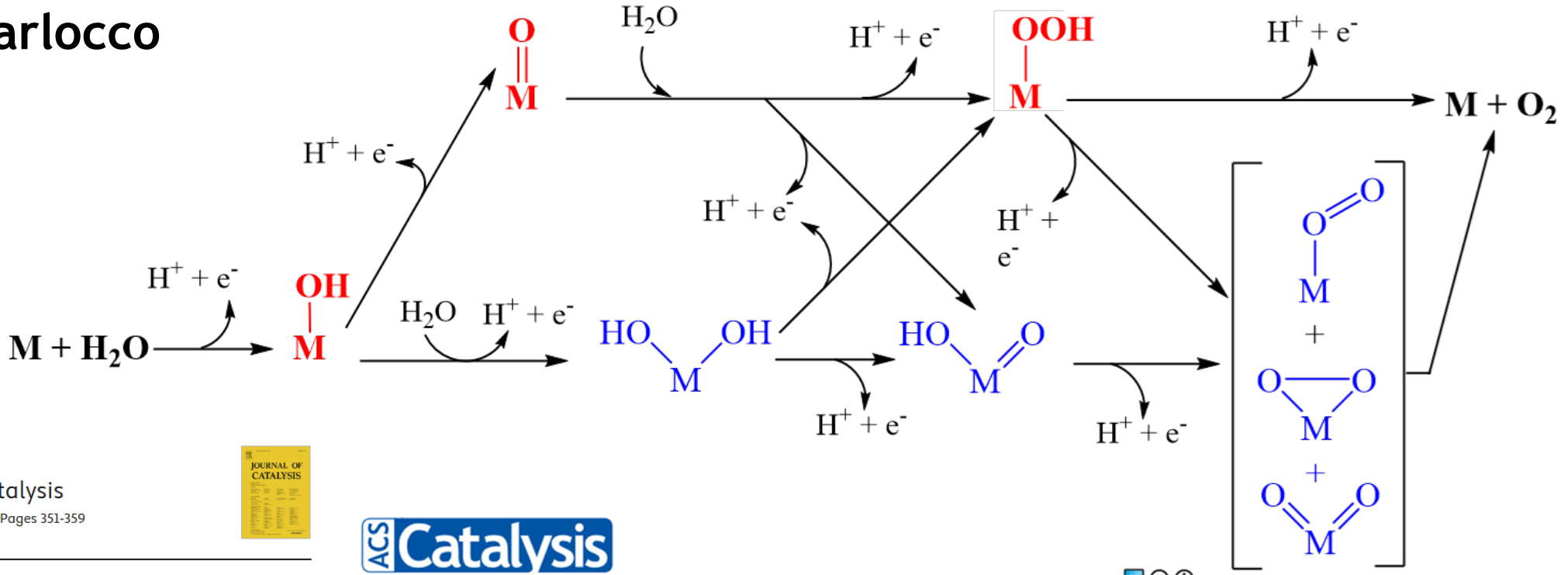
Reshaping the Modelling Approach

Ilaria Barlocco



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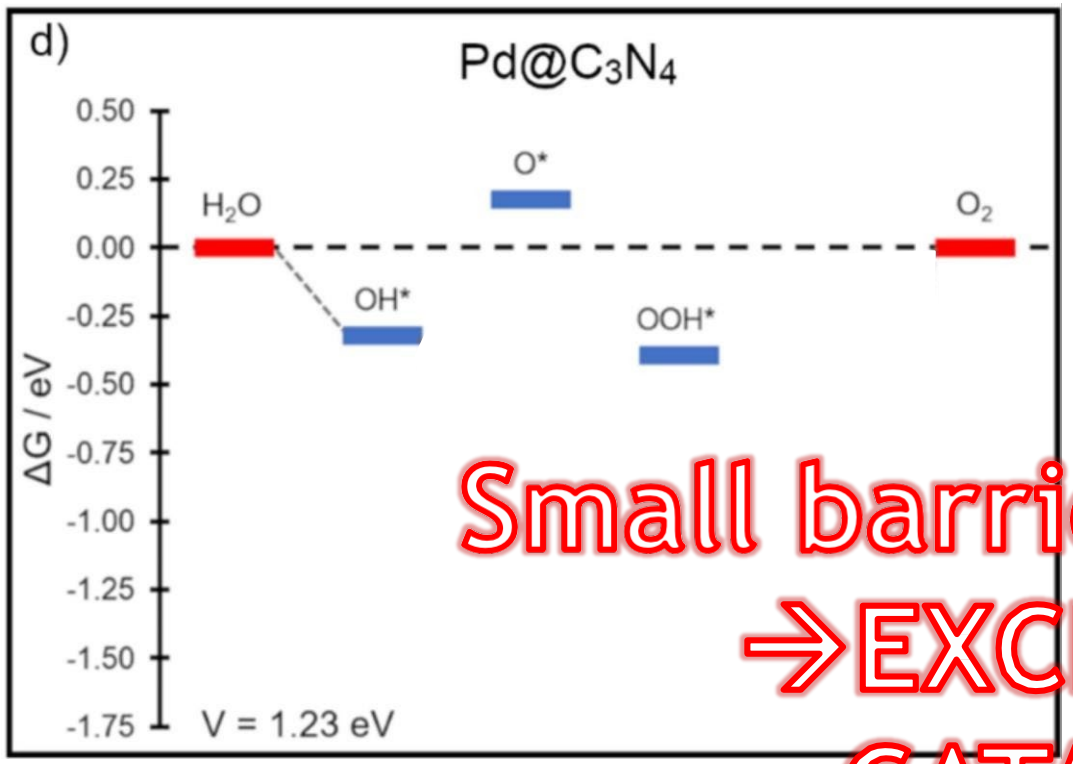
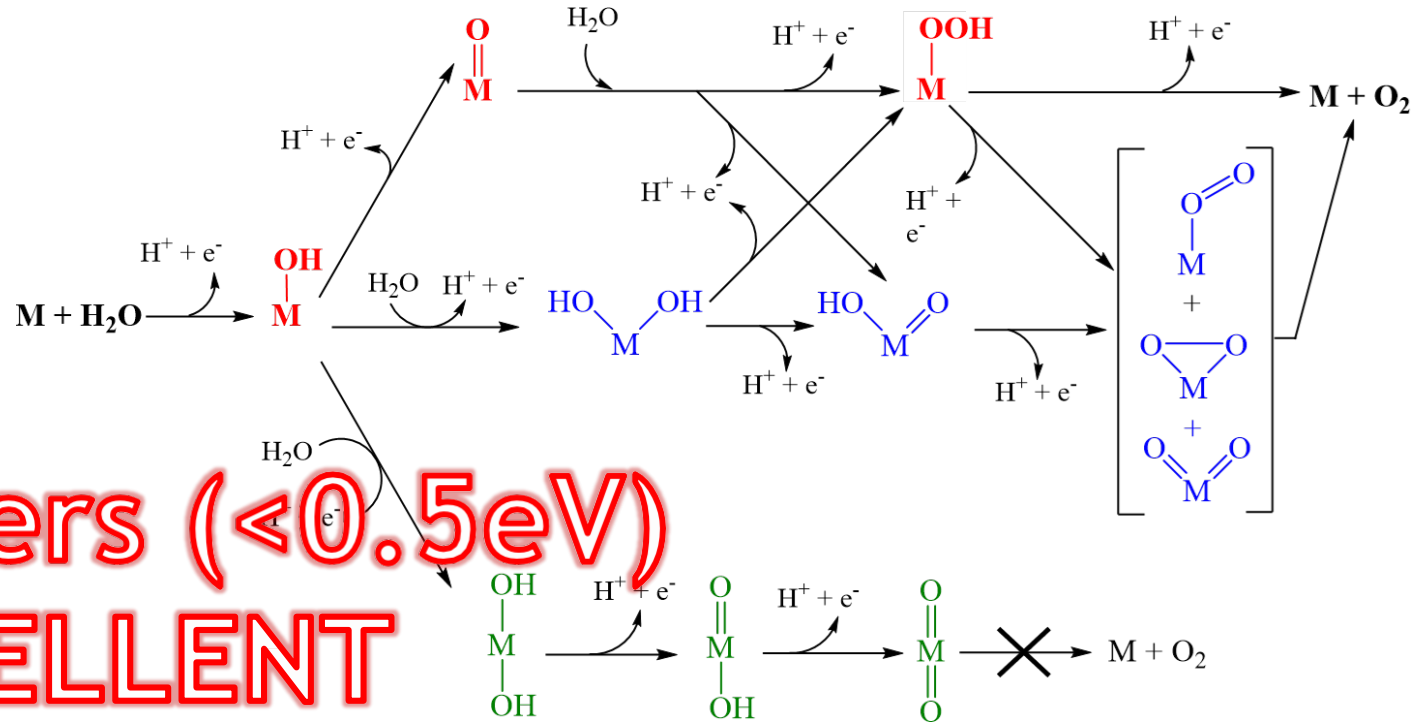
Superoxo and Peroxo Complexes on Single-Atom Catalysts: Impact on the Oxygen Evolution Reaction

Luis A. Cipriano, Giovanni Di Liberto,* and Gianfranco Pacchioni

Reshaping the Modelling Approach





Small barriers (<0.5eV)
→EXCELLENT CATALYST

I. Barlocco, L.A. Cipriano, G. Di Liberto, G. Pacchioni *J. Catal*, **417**, 351 (2023)

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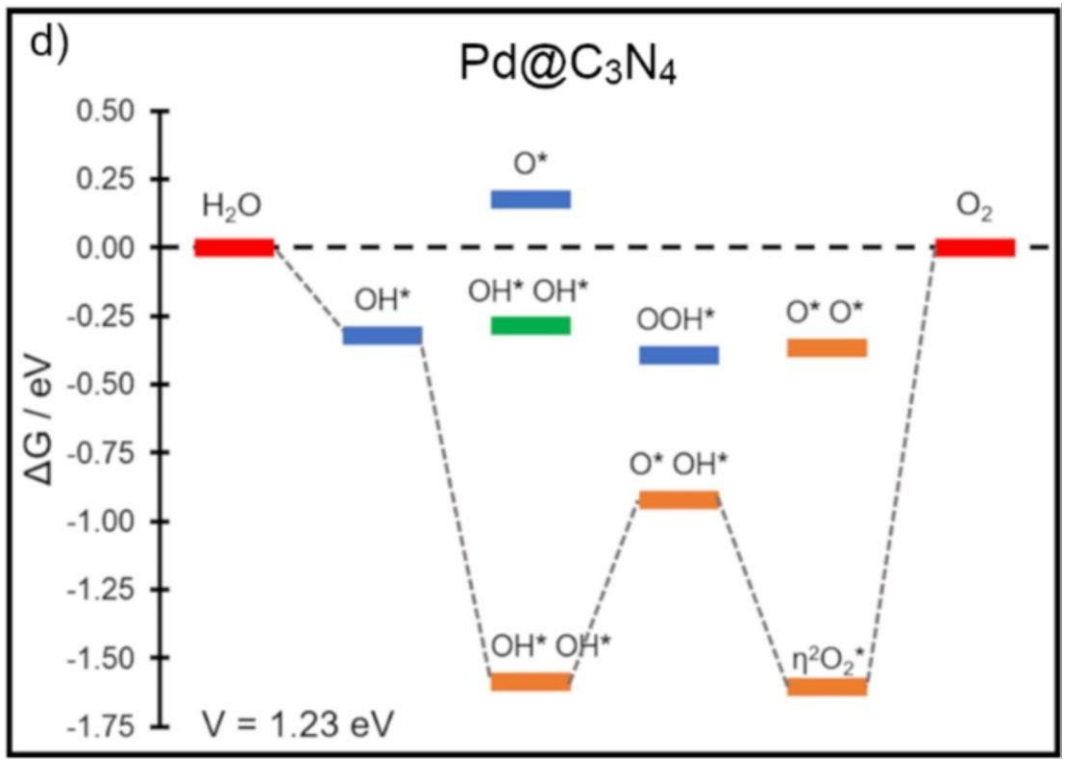

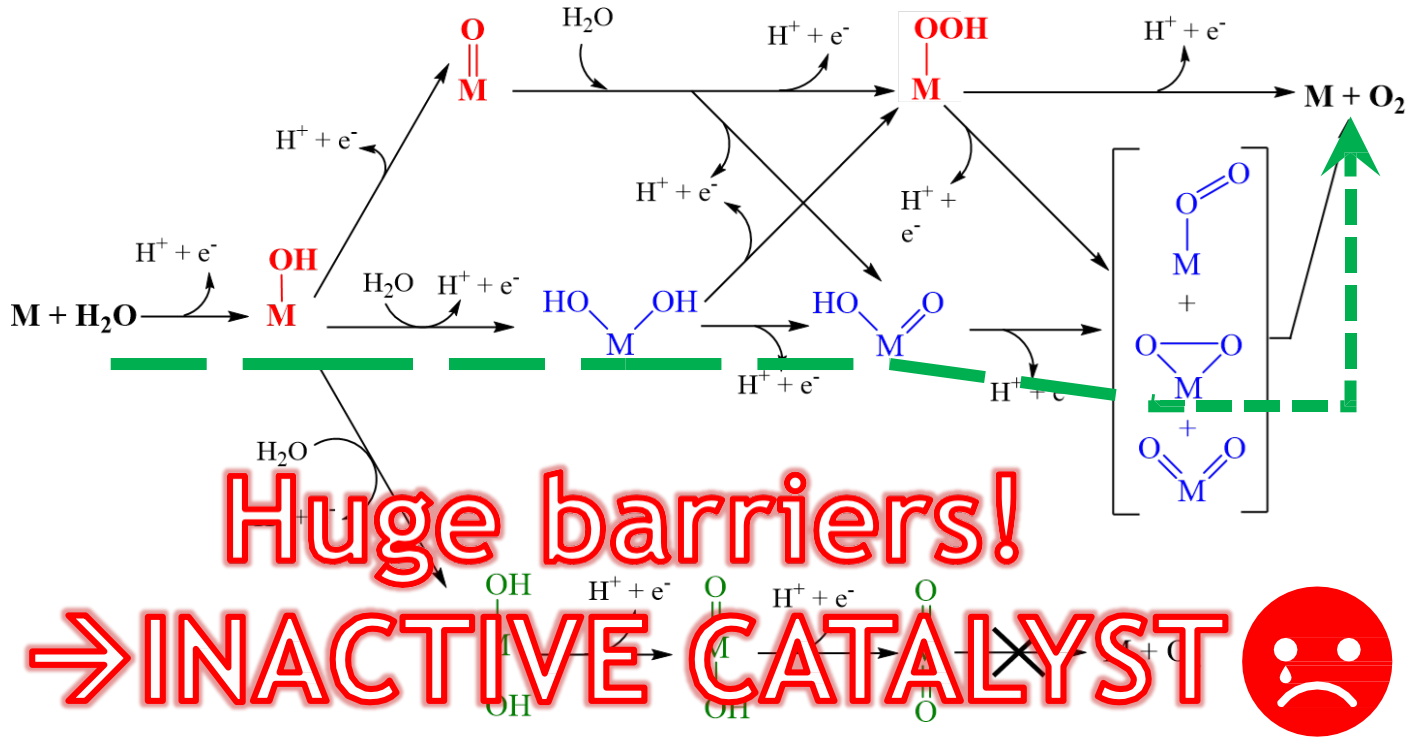

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What about the stability in electrochemical conditions?

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CHEMICAL REVIEWS

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Single-Atom (Iron-Based) Catalysts: Synthesis and Applications

Baljeet Singh, Manoj B. Gawande,* Arun D. Kute, Rajender S. Varma, Paolo Fornasiero, Peter McNeice, Rajenahally V. Jagadeesh, Matthias Beller,* and Radek Zbořil*

Cite This: *Chem. Rev.* 2021, 121, 13620−13697 Read Online

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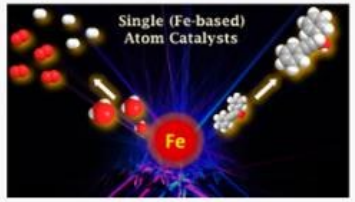
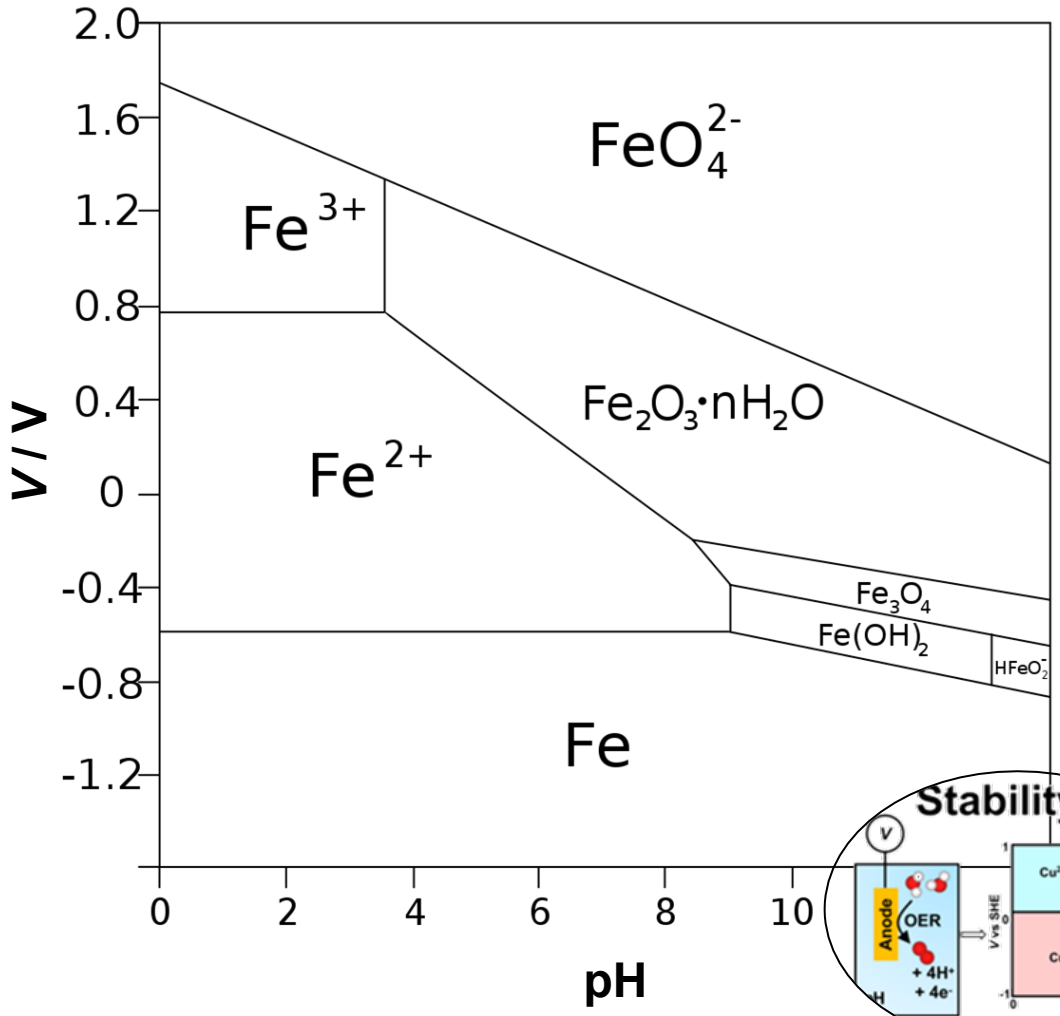
ABSTRACT: Supported single-metal atom catalysts (SACs) are constituted of isolated active metal centers, which are heterogenized on inert supports such as graphene, porous carbon, and metal oxides. Their thermal stability, electronic properties, and catalytic activities can be controlled via interactions between the single-metal atom center and neighboring heteroatoms such as nitrogen, oxygen, and sulfur. Due to the atomic dispersion of the active catalytic centers, the amount of metal required for catalysis can be decreased, thus offering new possibilities to control the selectivity of a given transformation as well as to improve catalyst turnover frequencies and turnover numbers. This review aims to comprehensively summarize the synthesis of Fe-SACs with a focus on anchoring single atoms (SA) on carbon/graphene supports. The characterization of these advanced materials using various spectroscopic techniques and their applications in diverse research areas are described. When applicable, mechanistic investigations conducted to understand the specific behavior of Fe-SACs-based catalysts are highlighted, including the use of theoretical models.





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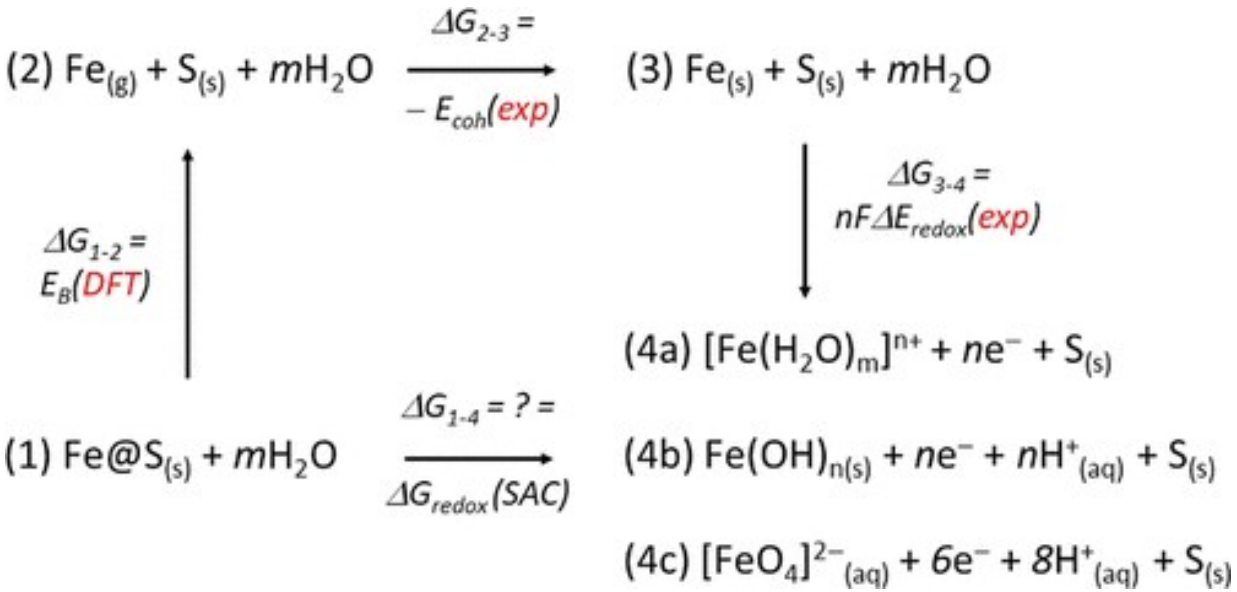
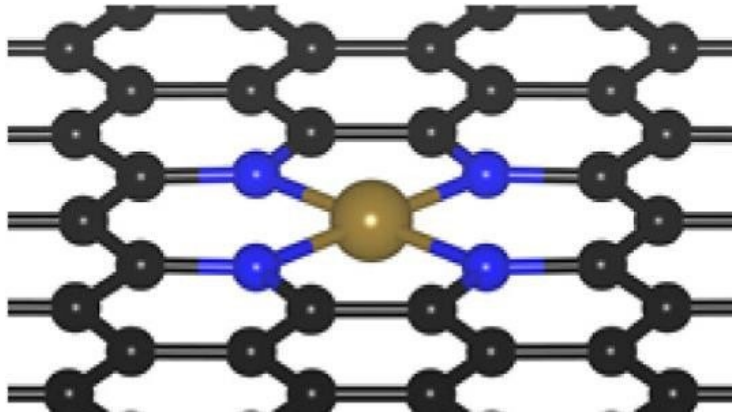
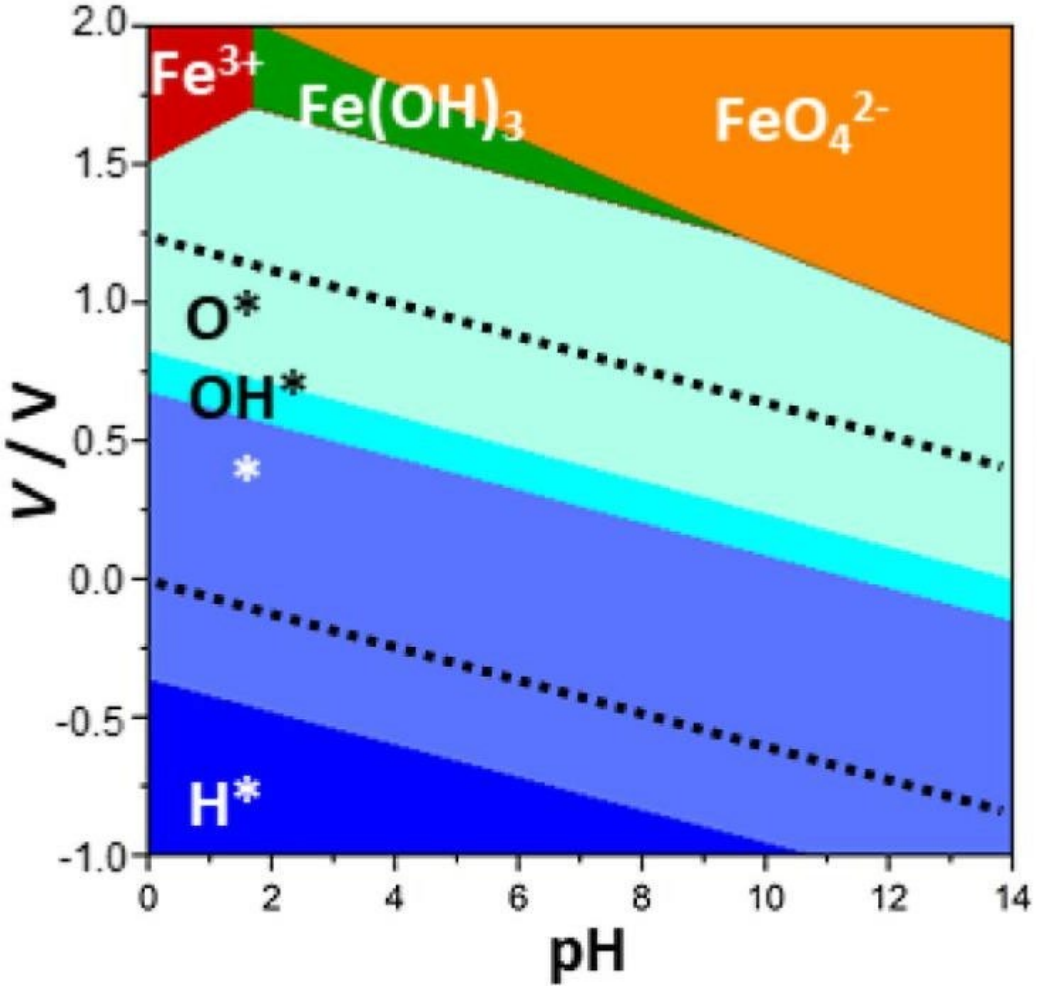
What about the stability in electrochemical conditions?







G. Di Liberto, L. Giordano, G. Pacchioni *ACS Catal.* **14**, 45 (2023)

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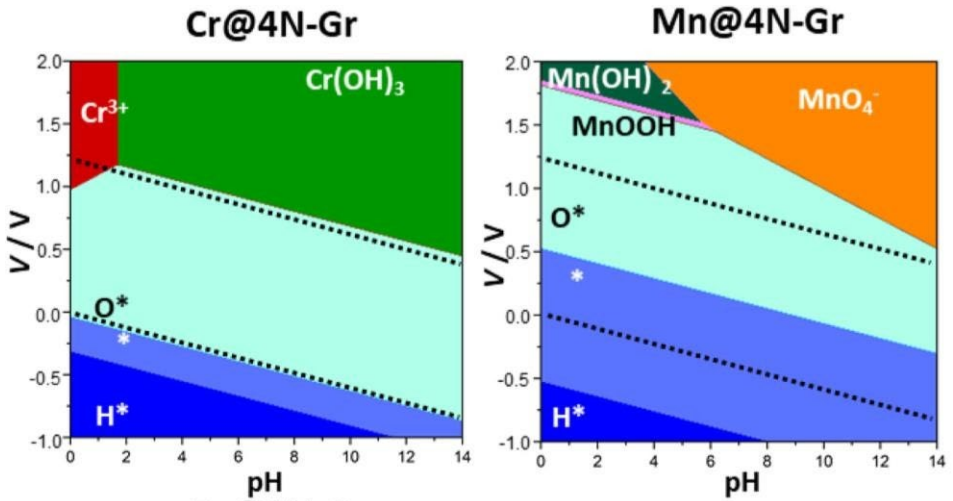

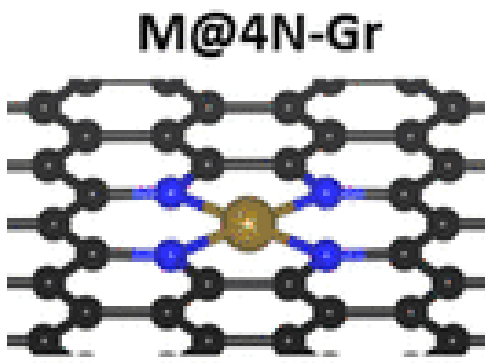

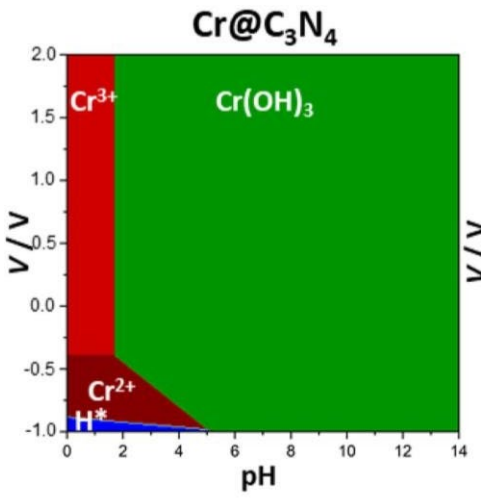

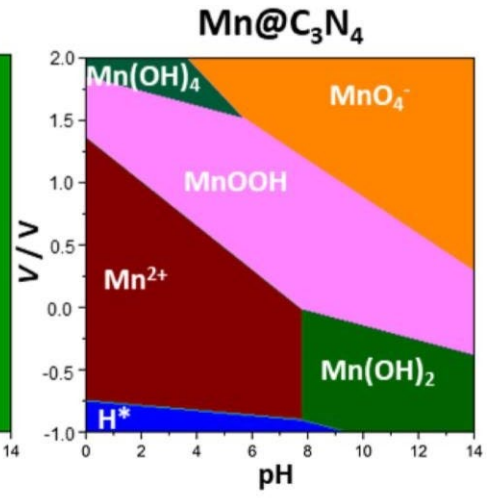

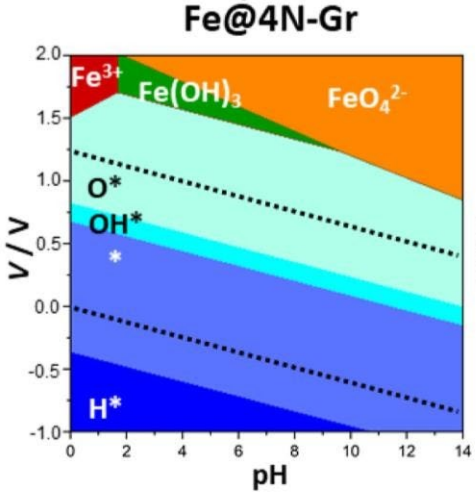

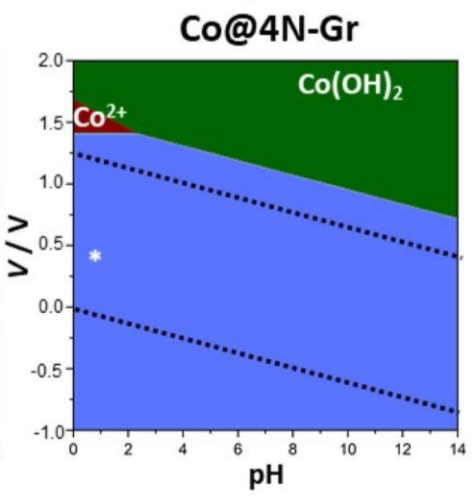

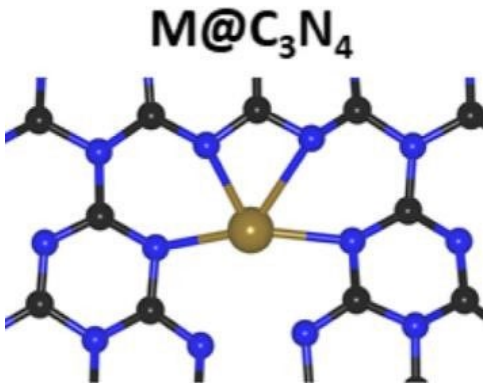

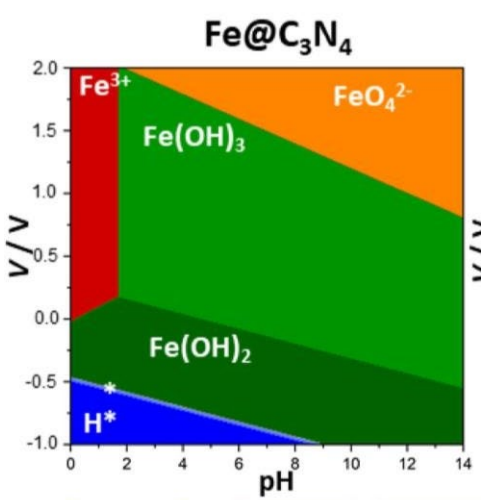

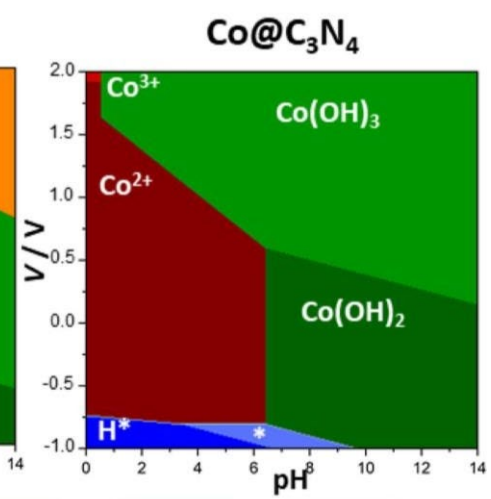

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Interplaying Theory and Experiment

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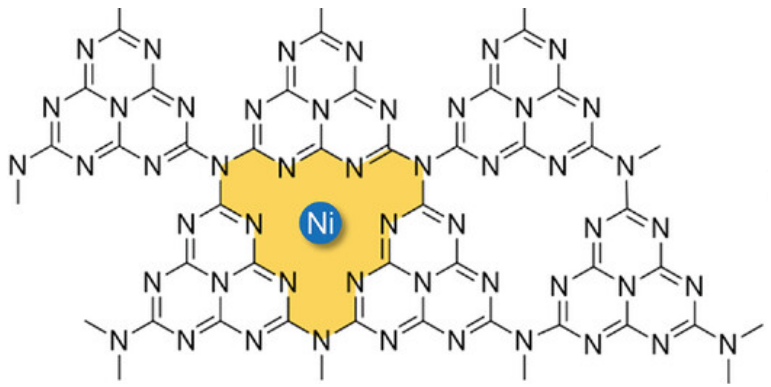
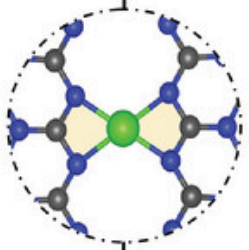
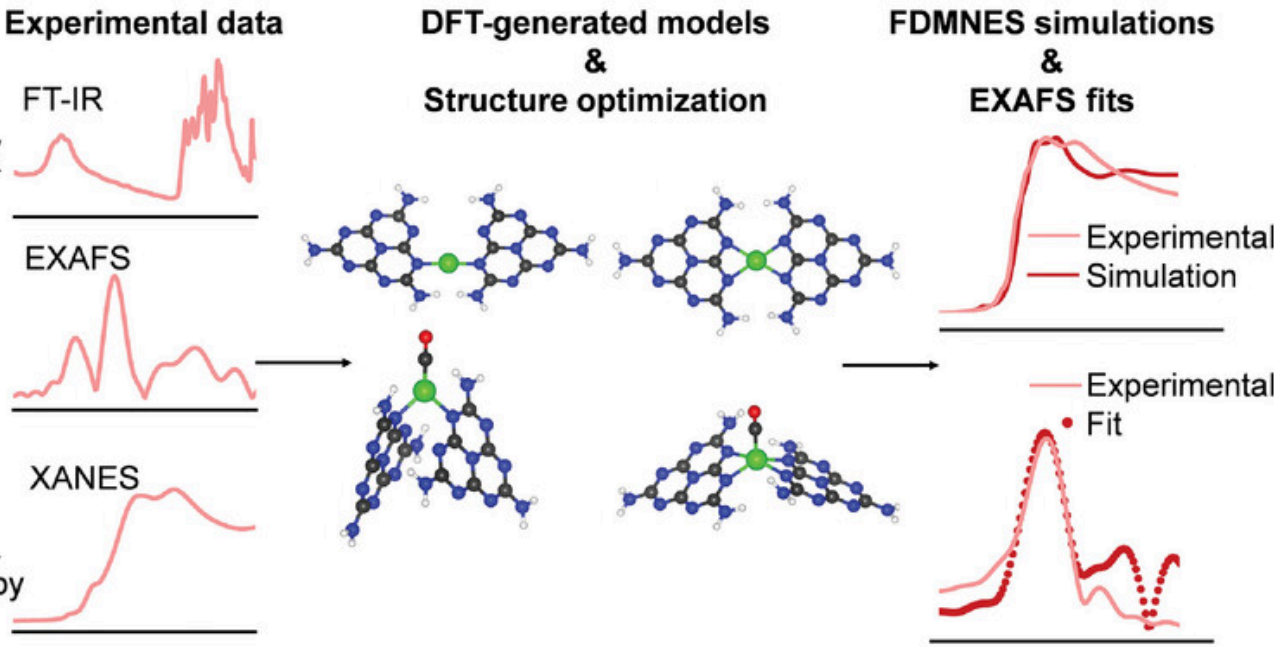


Shuai Xu





RESEARCH ARTICLE

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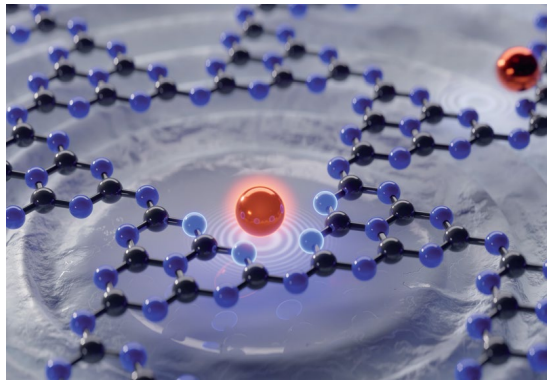
Resolving the Nanostructure of Carbon Nitride-Supported Single-Atom Catalysts



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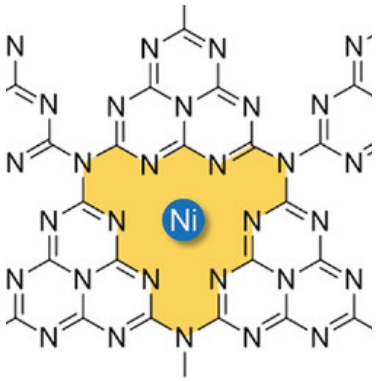
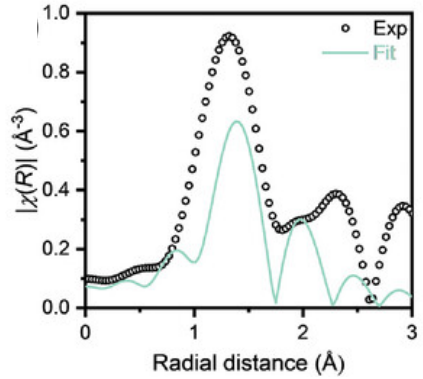
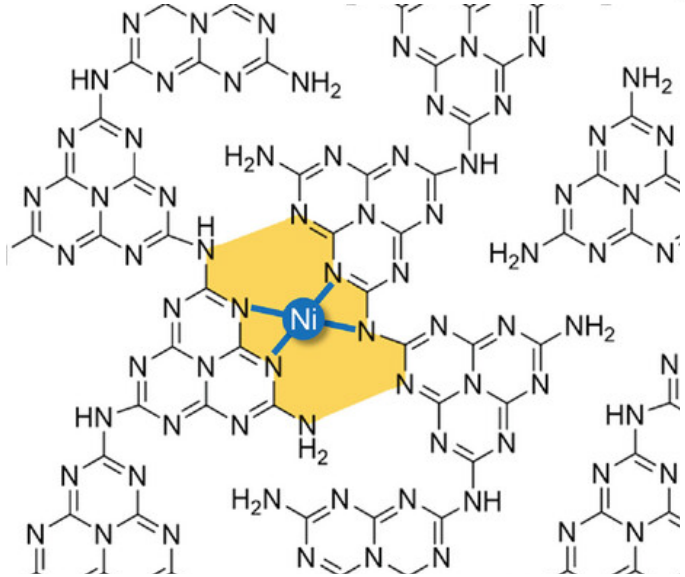
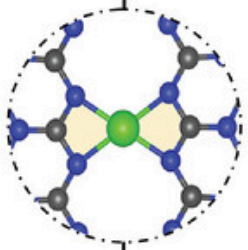








IR spectroscopy

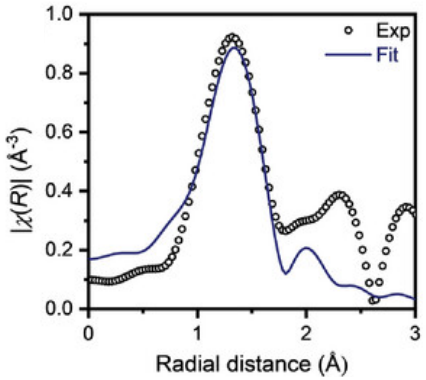
X-ray spectroscopy

Experimental data

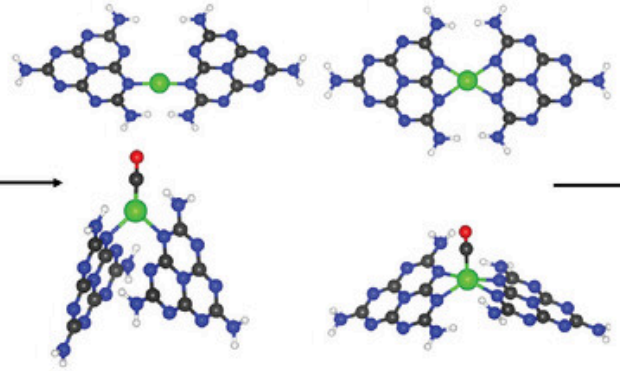
FT-IR

EXAFS

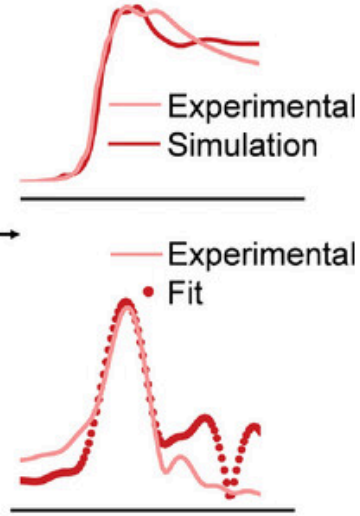
XANES



DFT-generated models & Structure optimization



FDMNES simulations & EXAFS fits



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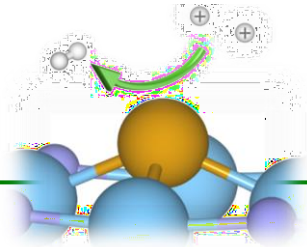
Application: The Case of Titanium Nitride



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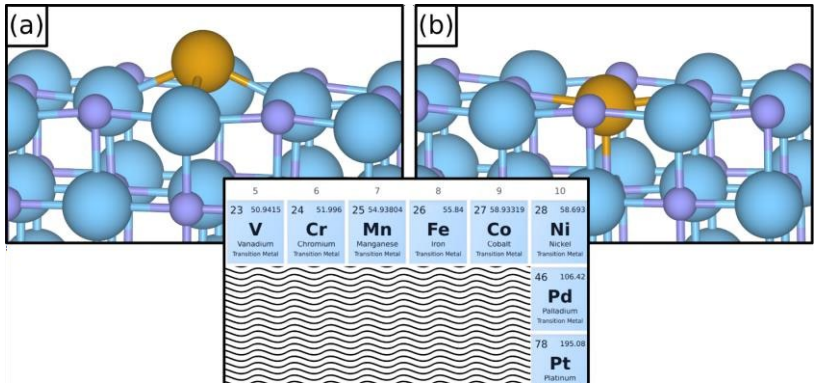
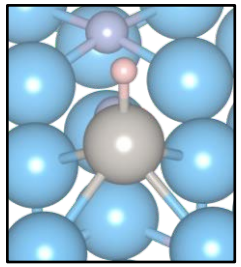


CONVENTIONAL INTERMEDIATE



12 good catalyst out of 16

Clara Saetta

RESEARCH ARTICLE

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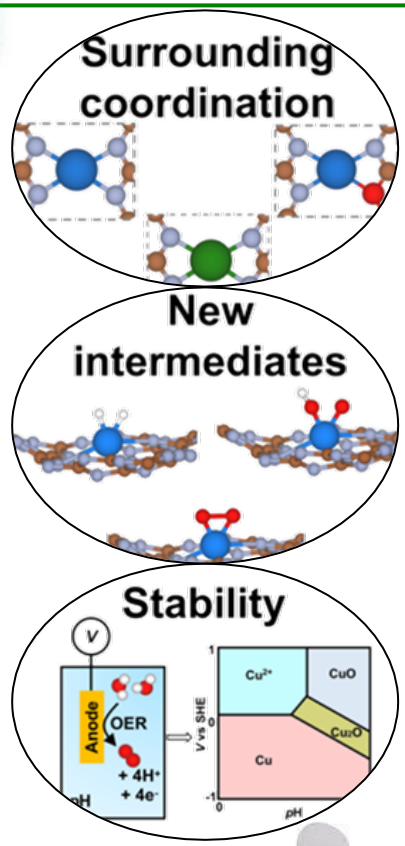
Key Ingredients for the Screening of Single Atom Catalysts for the Hydrogen Evolution Reaction: The Case of Titanium Nitride

Clara Saetta, Ilaria Barlocco, Giovanni Di Liberto, and Gianfranco Pacchioni**



Experiments: Pd, Pt

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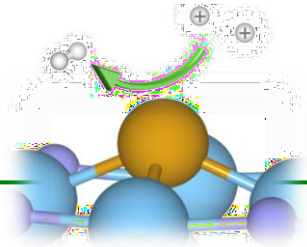

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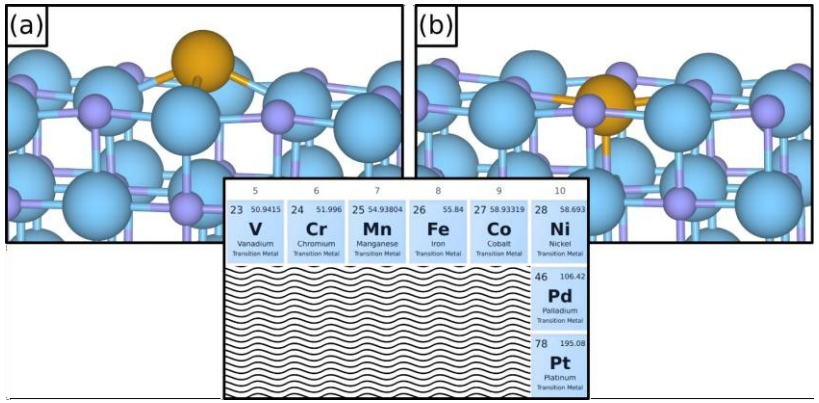

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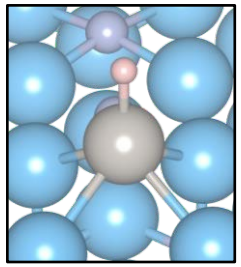

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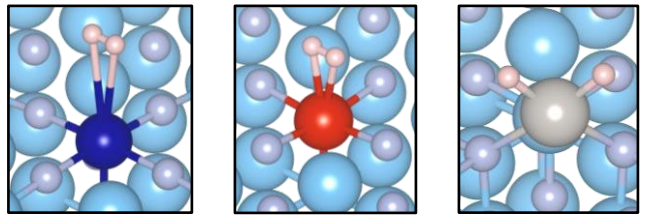
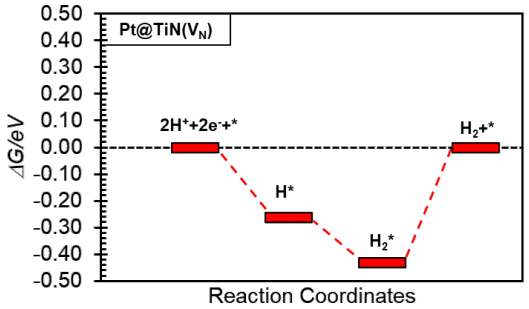
UNCONVENTIONAL INTERMEDIATES



H_{2phys} H_2* H*H*



The number of **potential candidates** is reduced to **6**

Experiments: Pd, Pt

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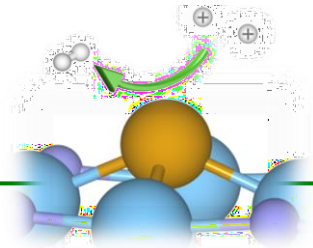

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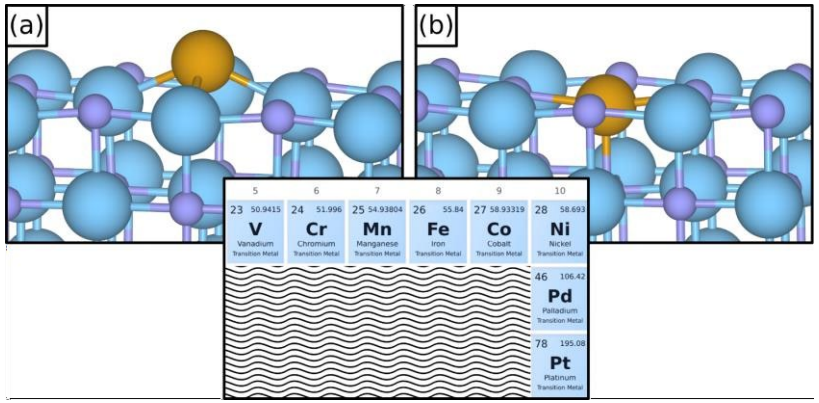

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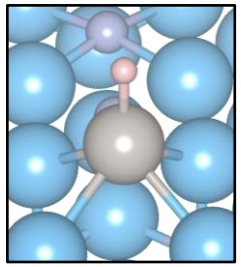

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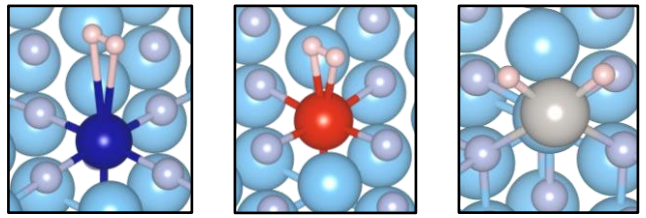
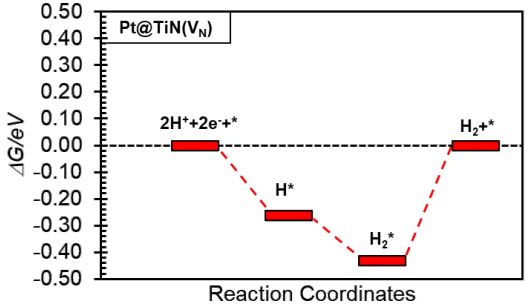


H_{2phys} H_2^* H^*H^*



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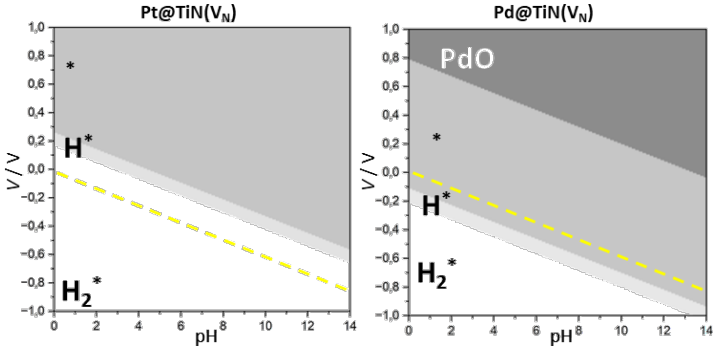
STABILITY

Pourbaix Diagrams



Only **Pt and Pd** are **stable** in **HER working conditions**

Experiments: Pd, Pt

C. Saetta, I. Barlocco, GDL, G. Pacchioni *Small*. **20**, 2401058 (2024)

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Single-Atoms on Goldene

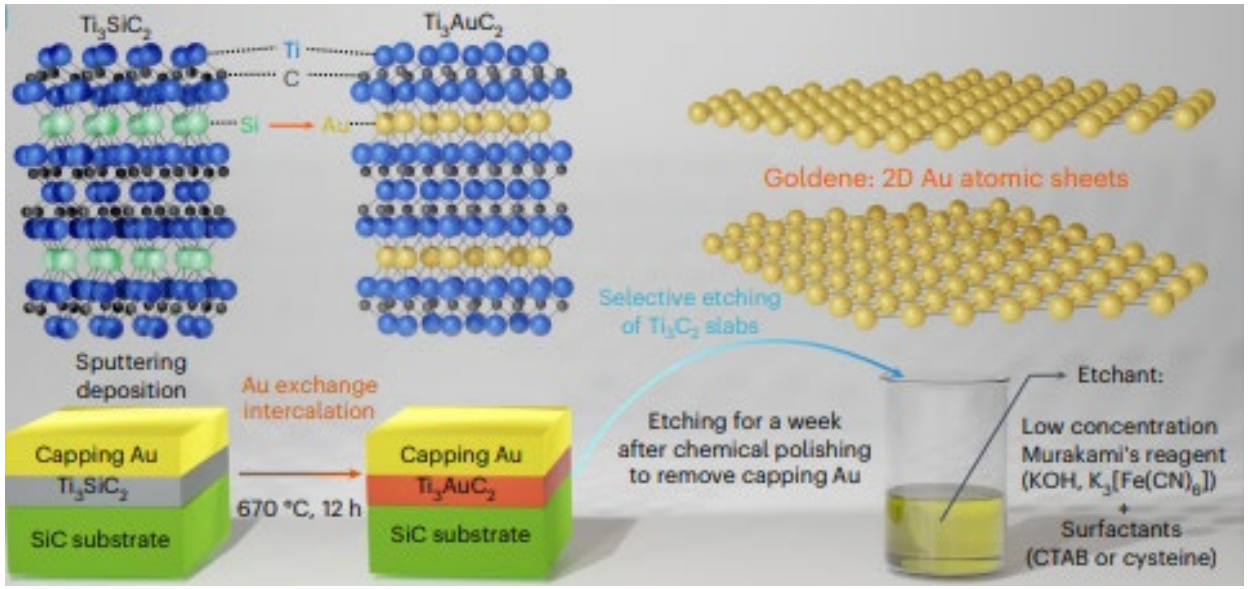
COST CA18234

nature synthesis

Article

https://doi.org/10.1038/s44160-024-00518-4

Synthesis of goldene comprising single-atom layer gold



Elisabetta

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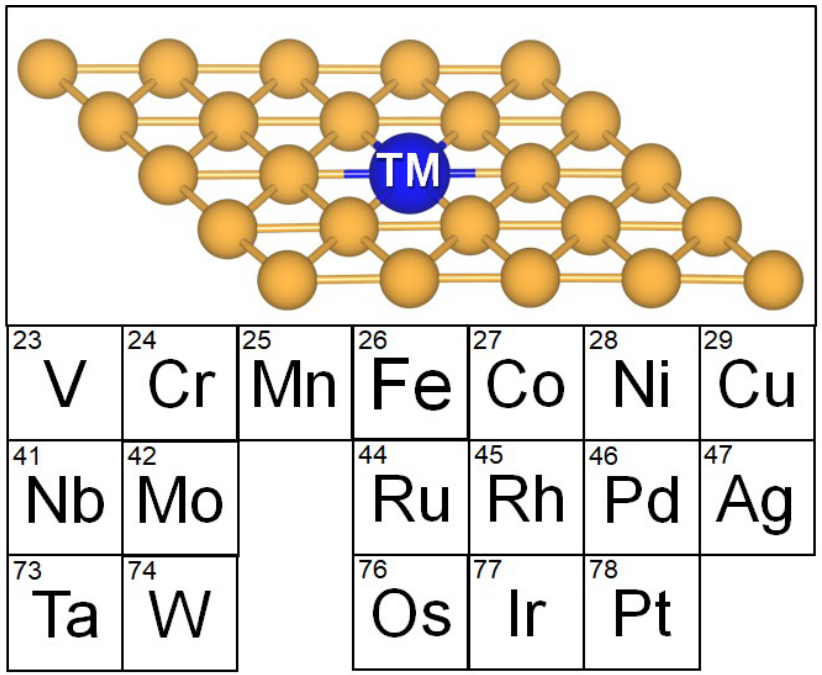

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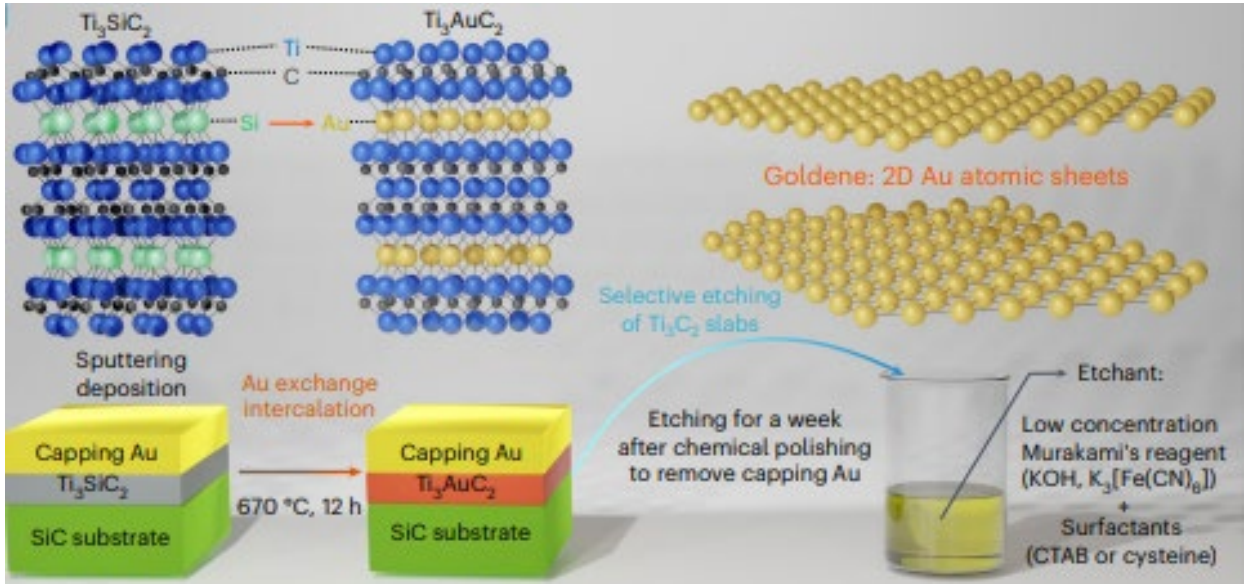
Research Article

Single-Atom Catalysts on Goldene

Silvia Picello,[‖] Elisabetta Inico,[‖] Clara Saetta,[‖] Giovanni Di Liberto,* and Gianfranco Pacchioni



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Clara

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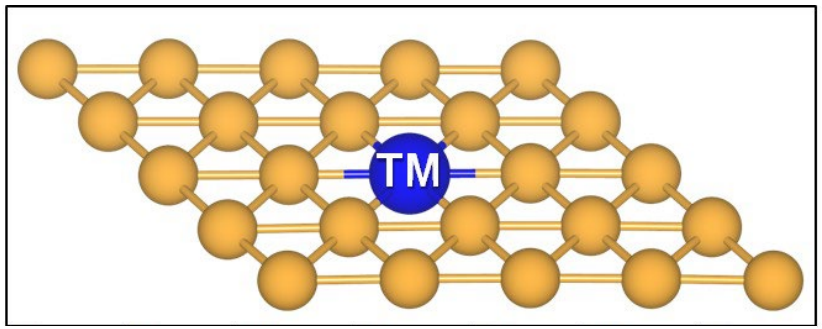

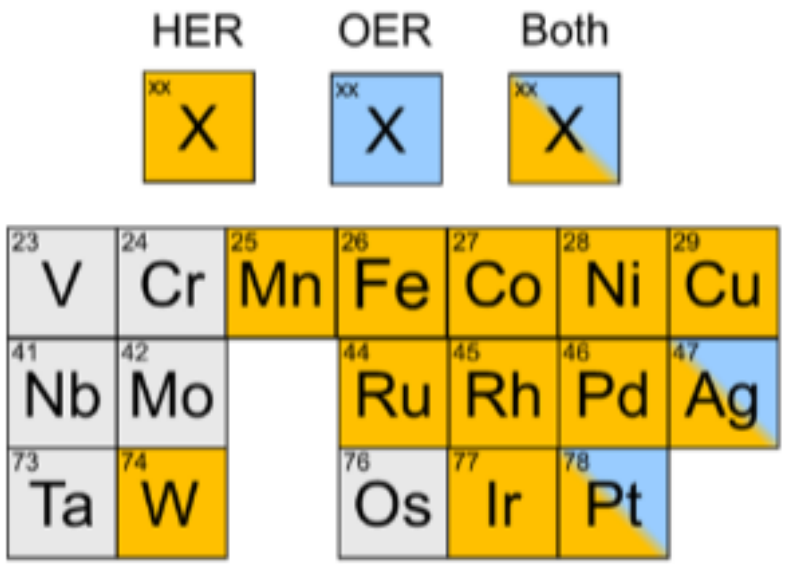

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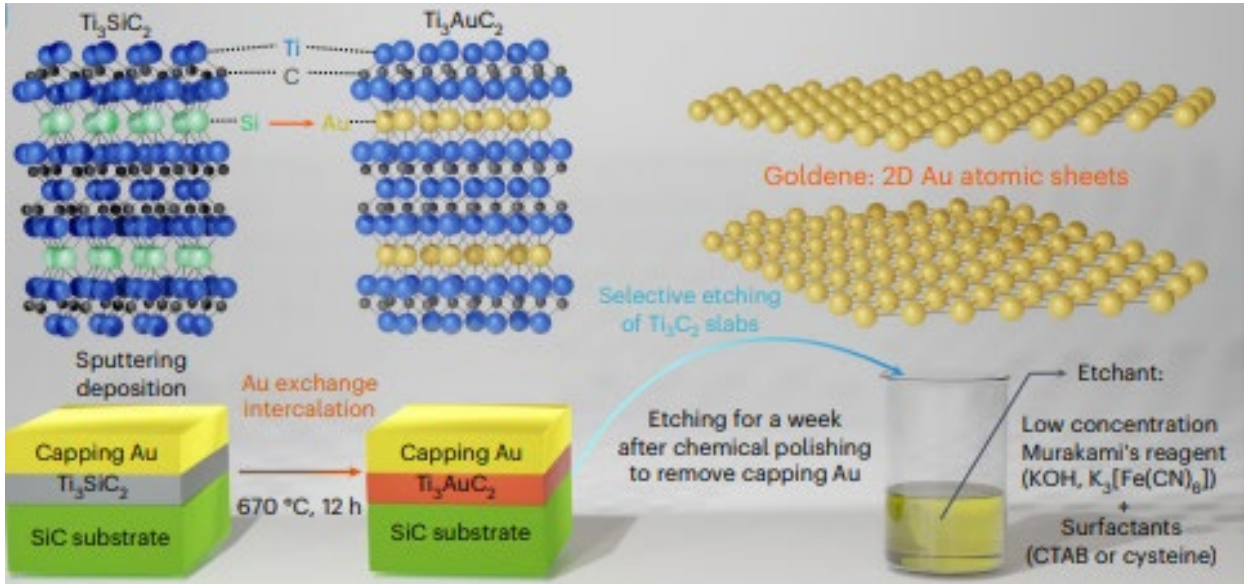

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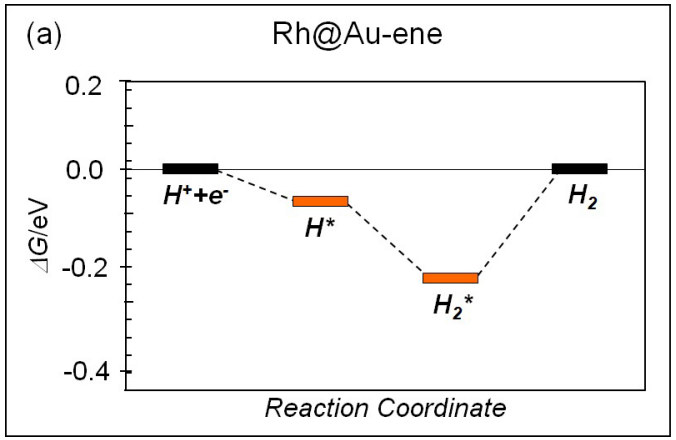
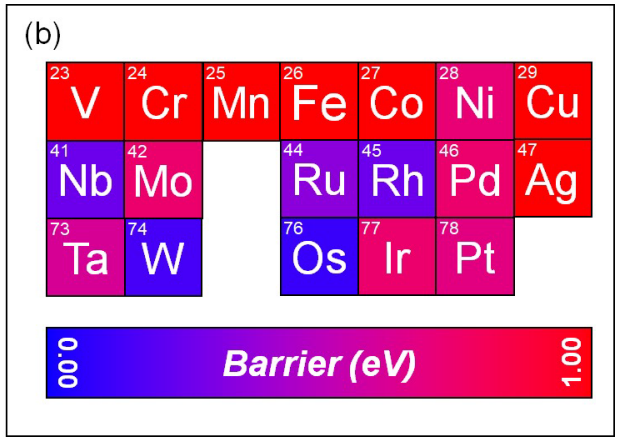
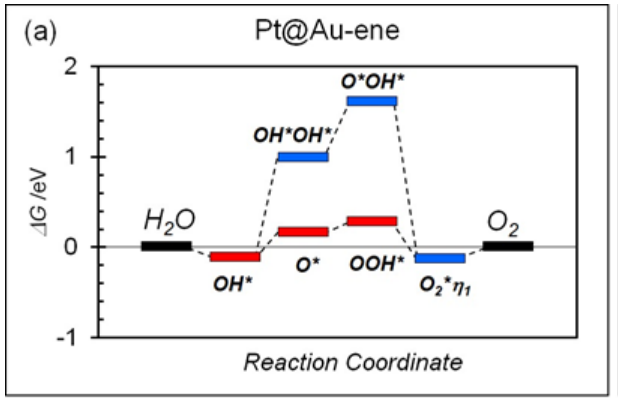
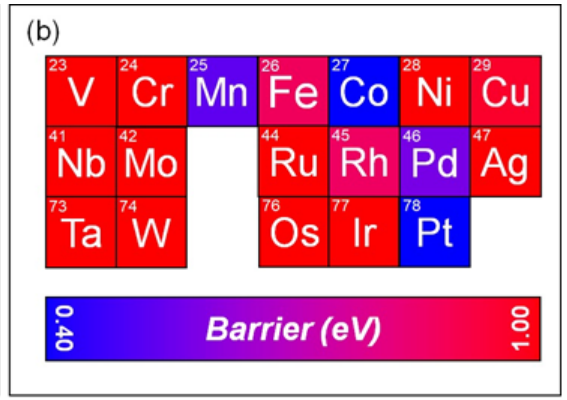
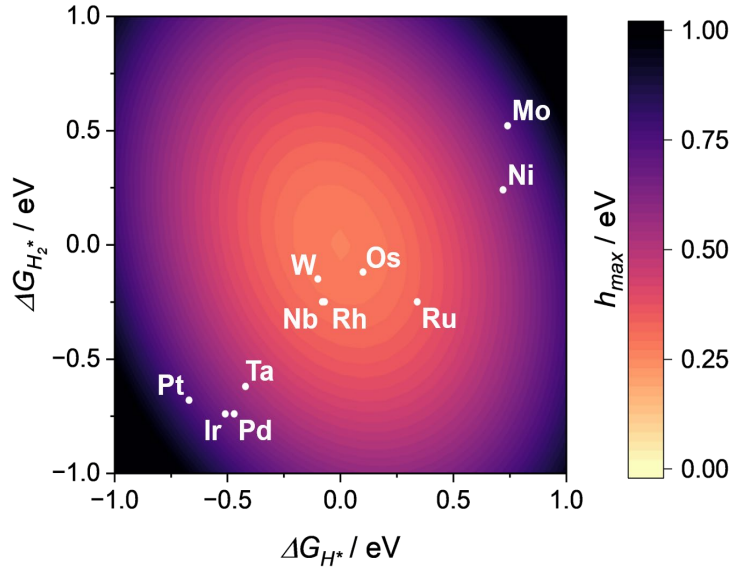








HER



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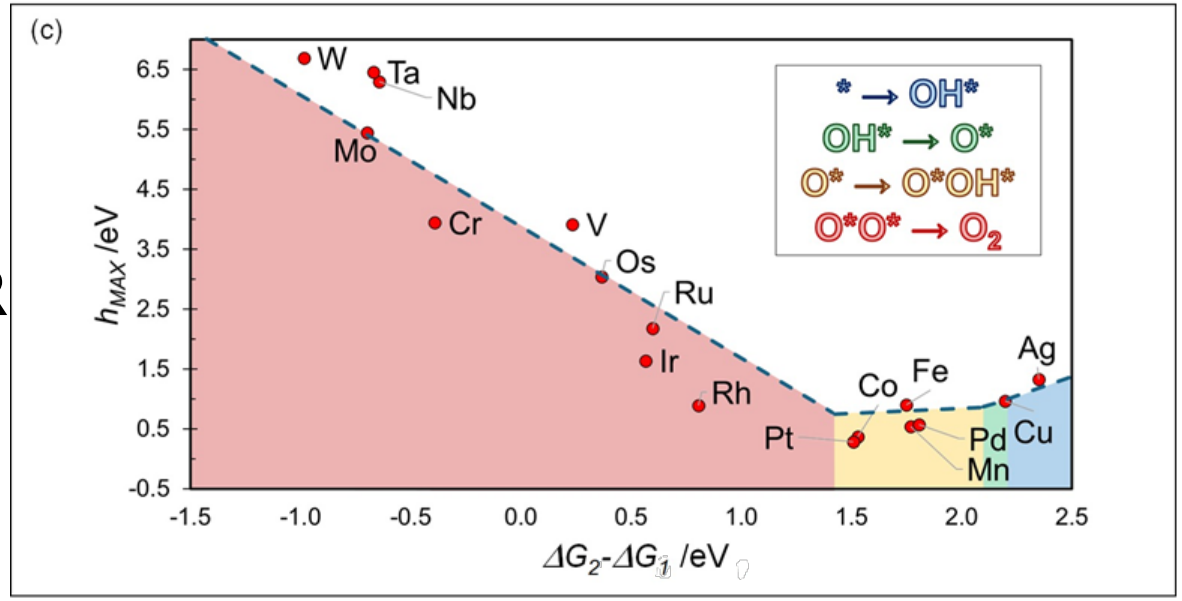

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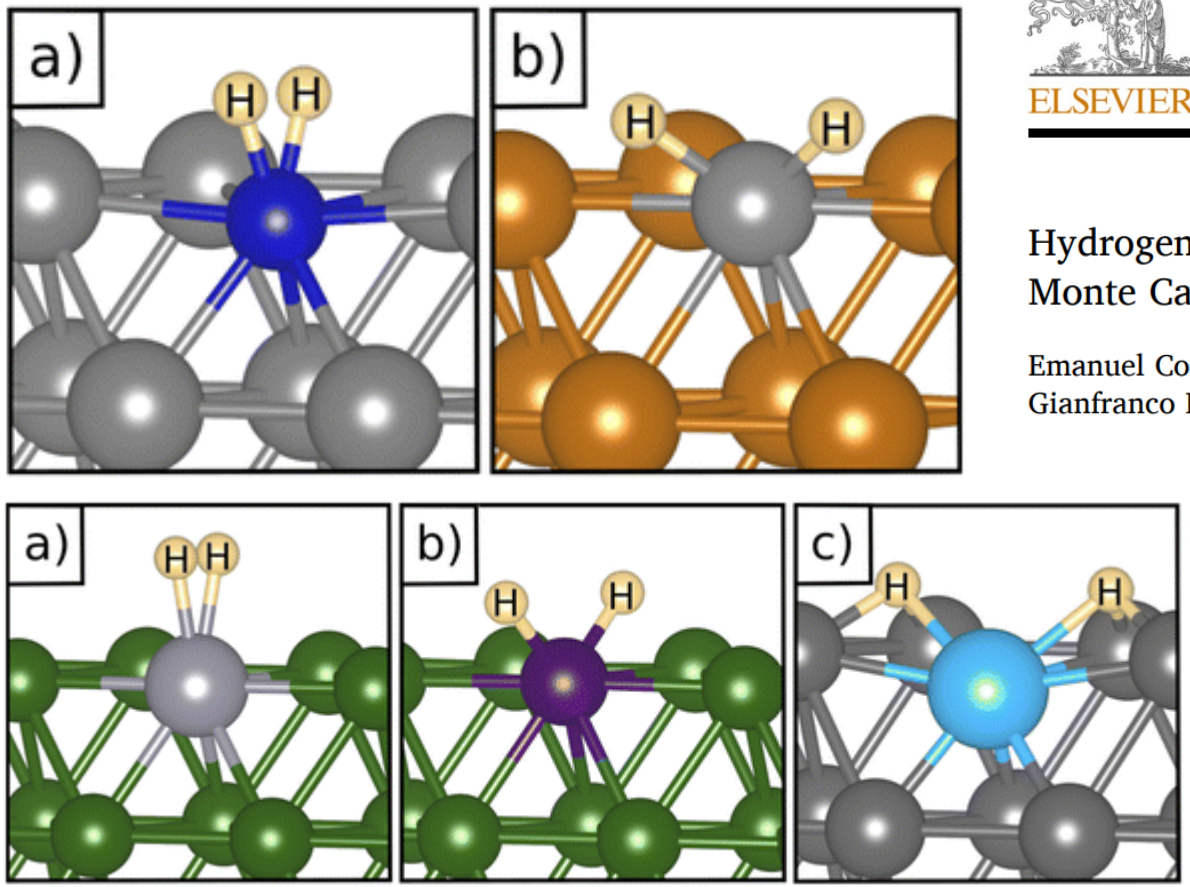
Combining DFT with KMC

COST CA18234

Co@Ag(111) Pt@Au(111)



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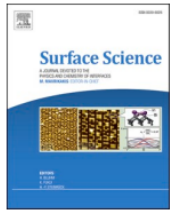

Check for updates

Hydrogen complexes on single-atom alloys: A combined DFT – Kinetic Monte Carlo study

Emanuel Colombi Manzi [a], Michail Stamatakis [b], Giovanni Di Liberto [a,*], Gianfranco Pacchioni [a,*]

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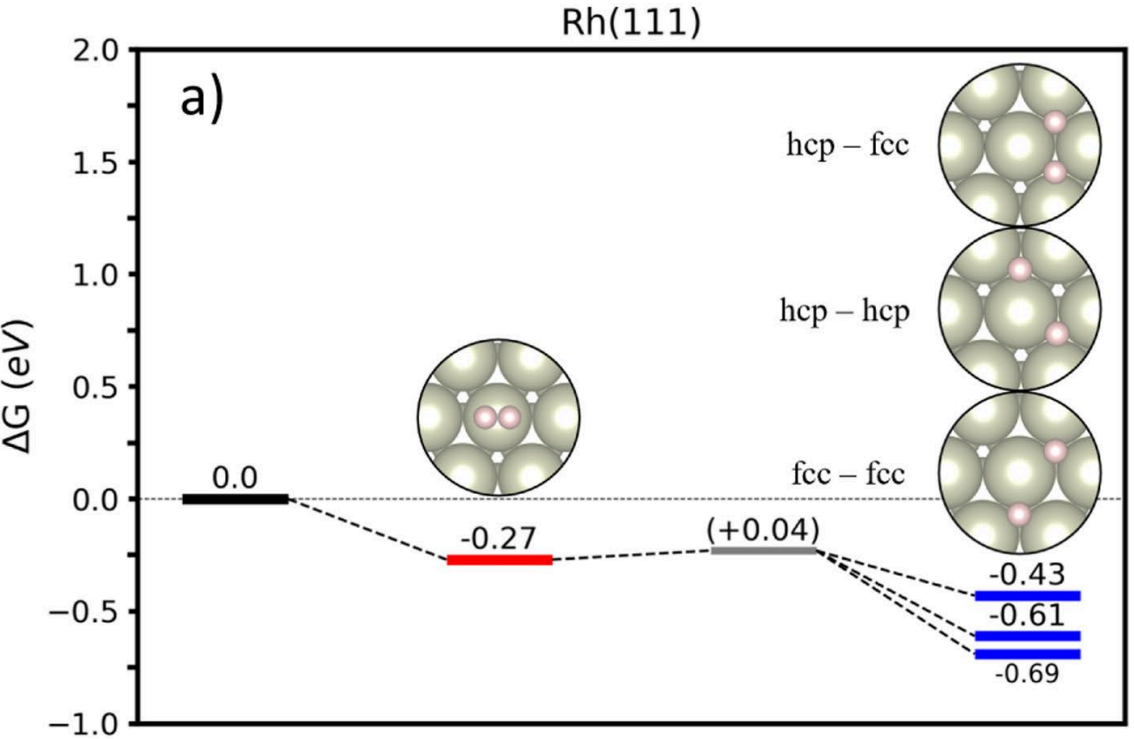
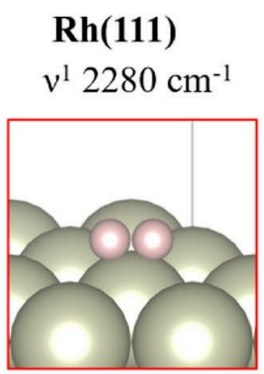




Rh(111)

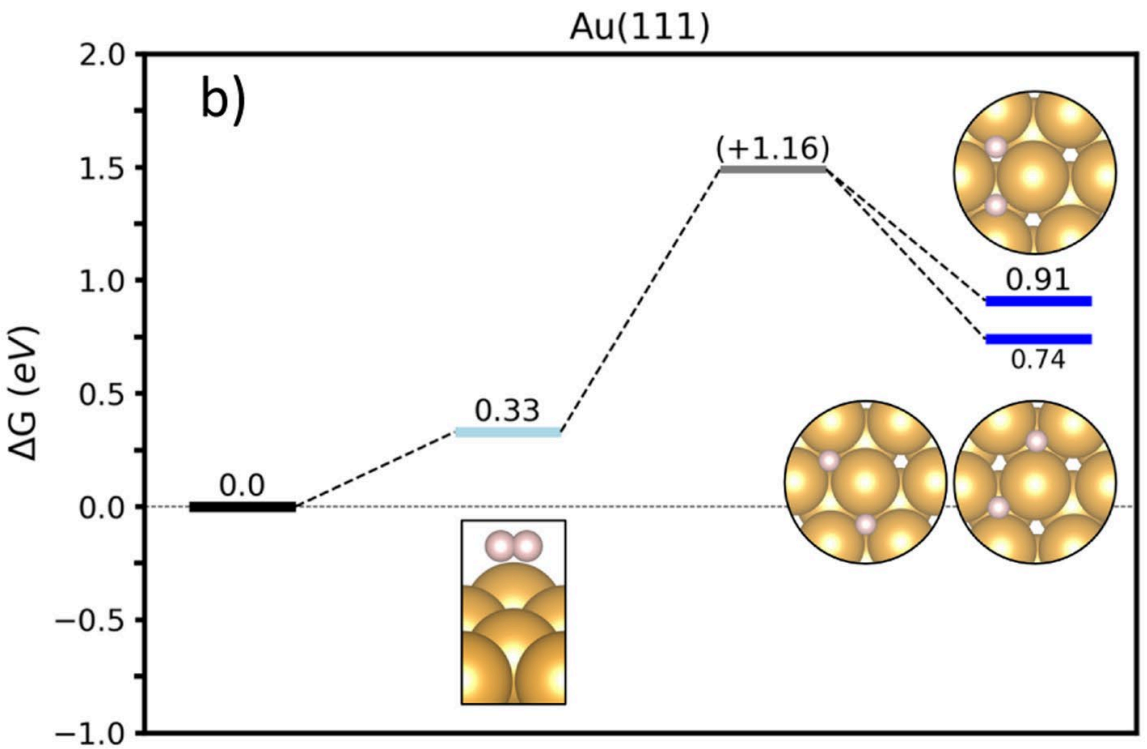
ν^1 2280 cm^{-1}

d H-H: **0.94** Å

d M-H_1: 1.69 Å

d M-H_2: 1.69 Å

ΔE = -0.68 eV



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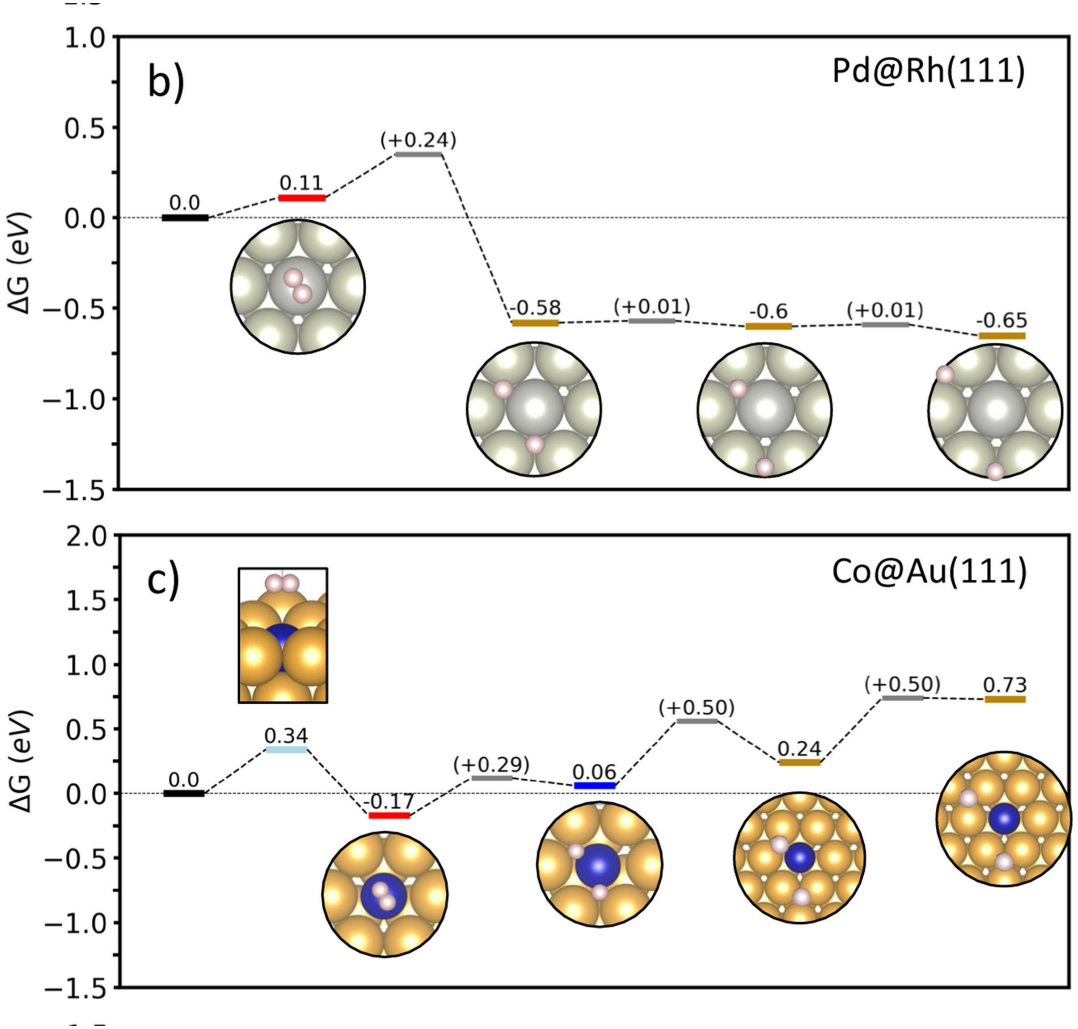

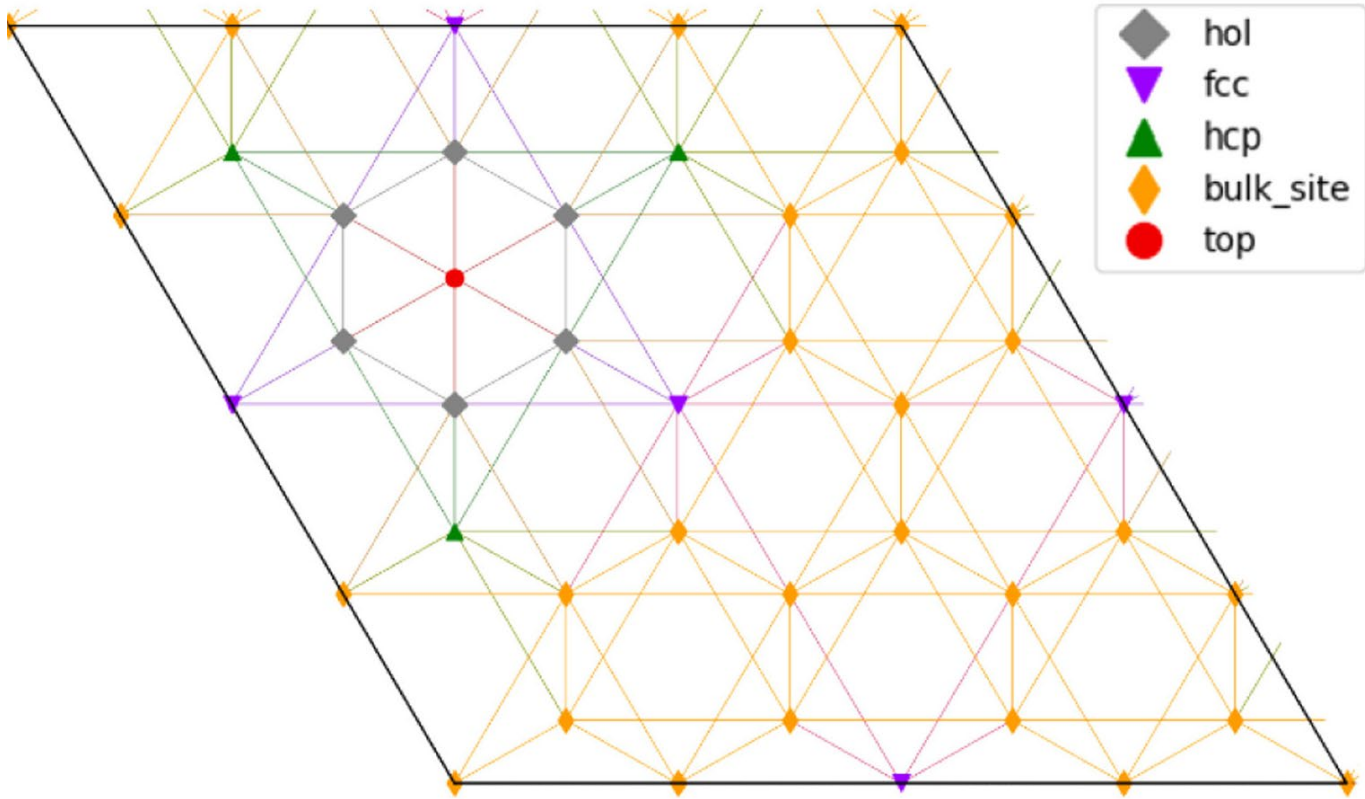

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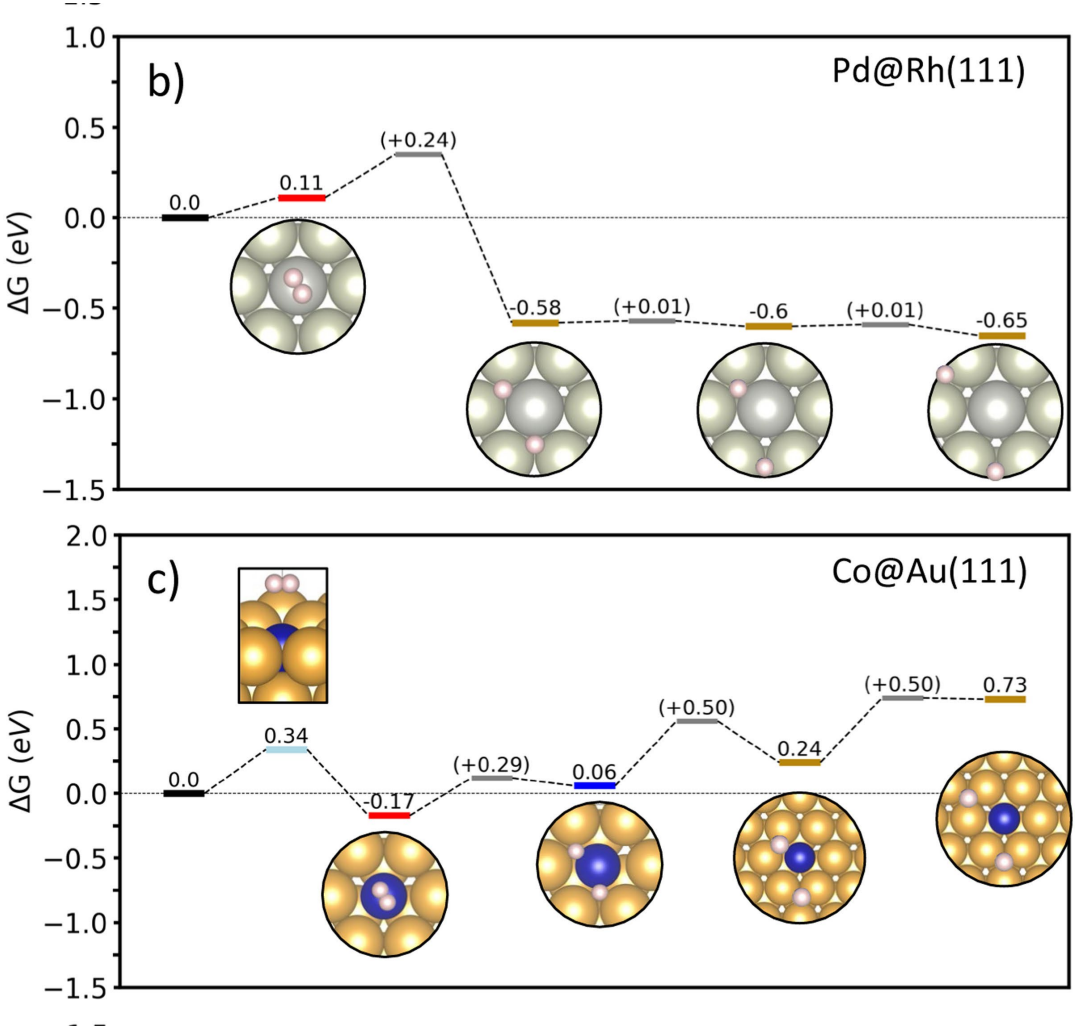

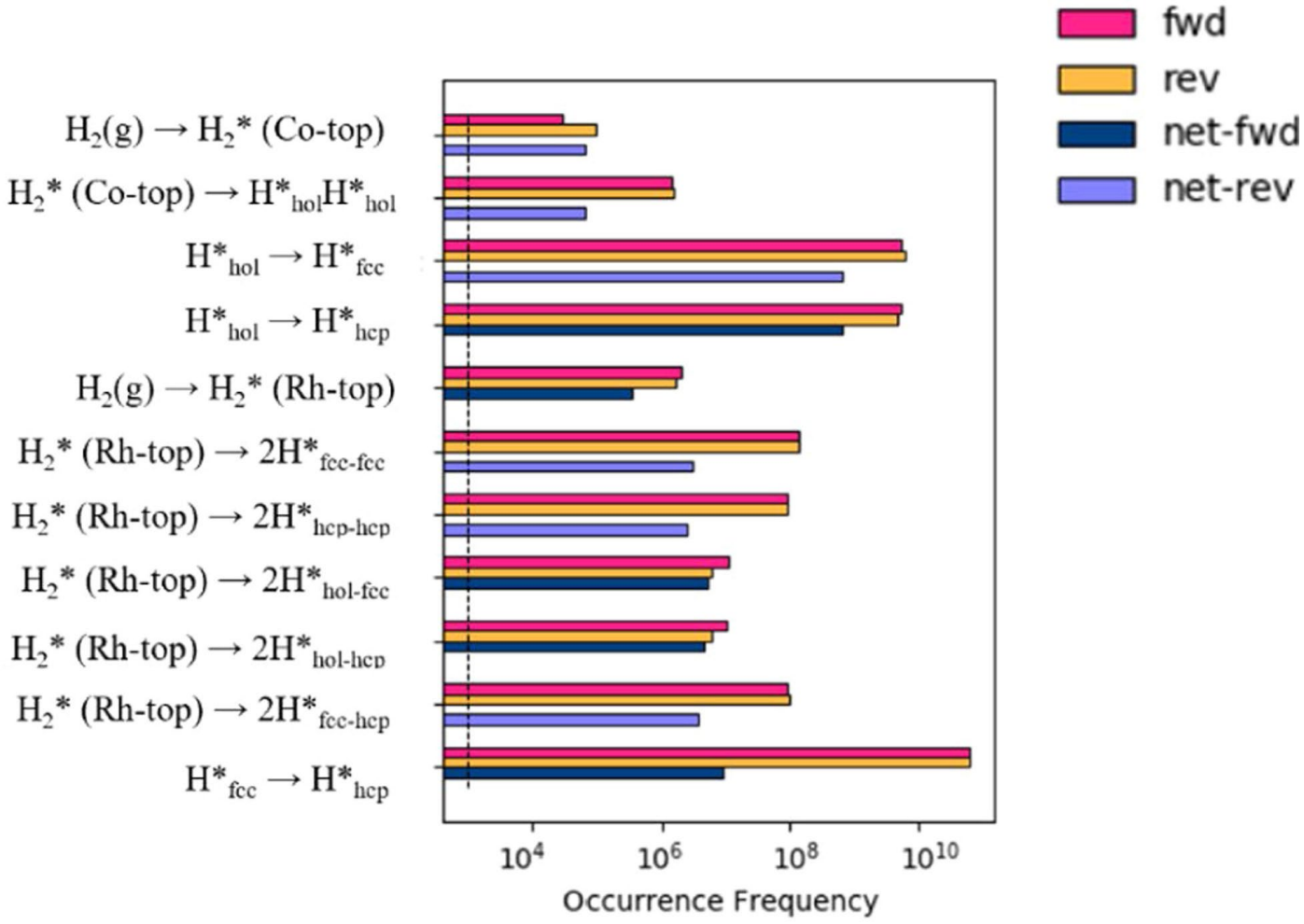

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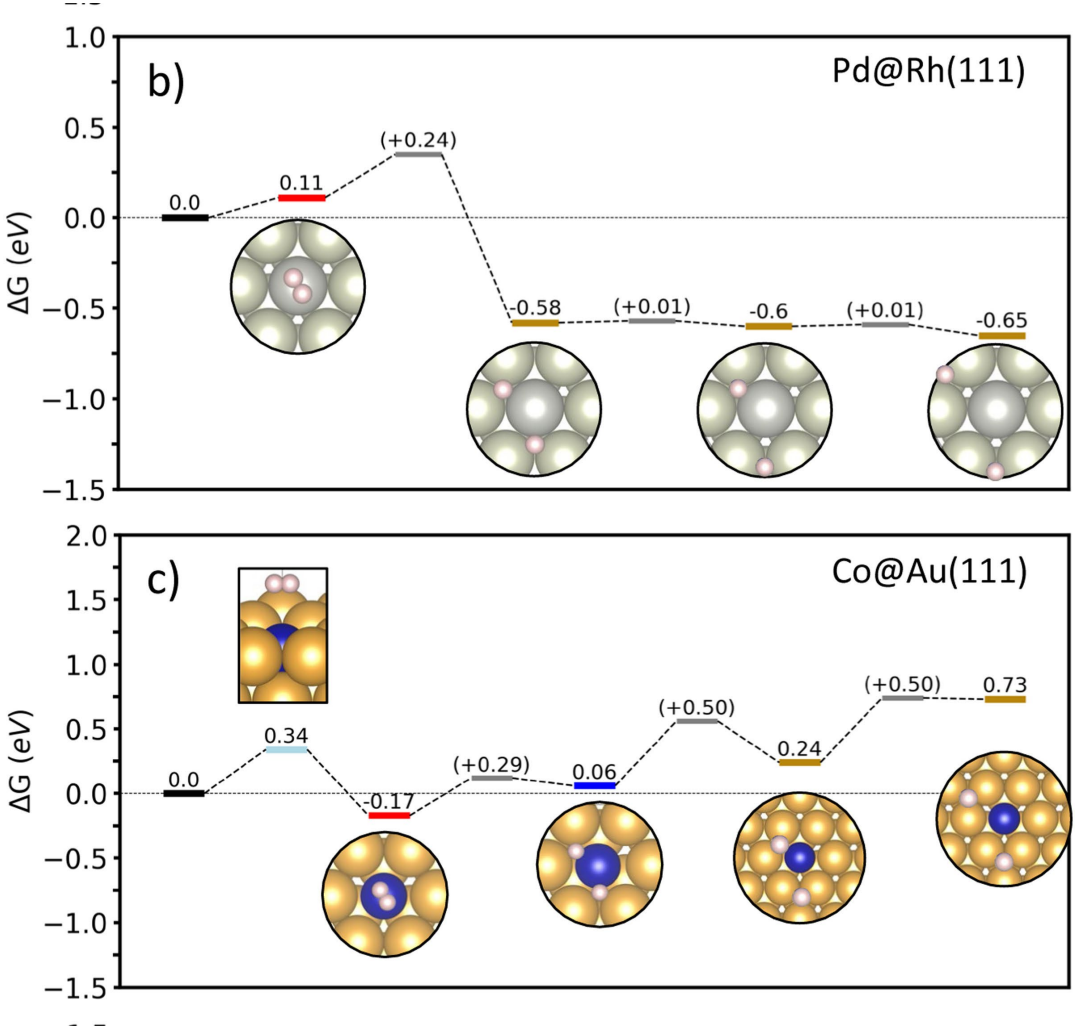

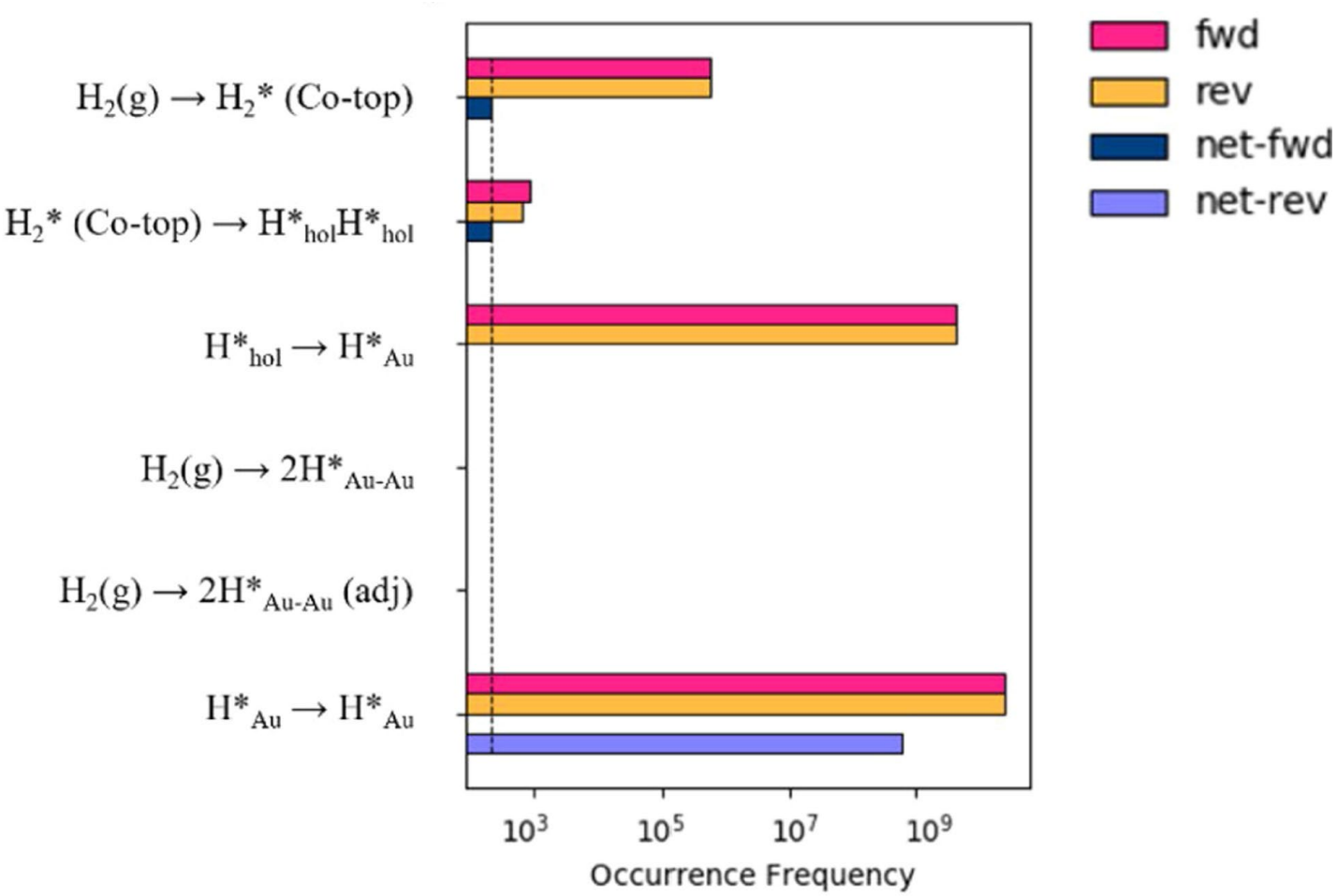

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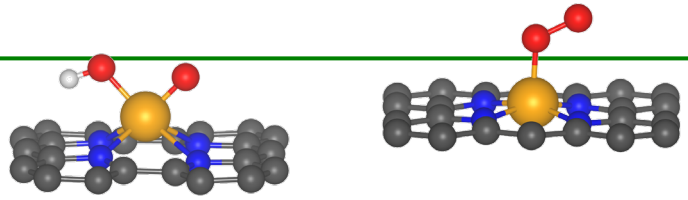
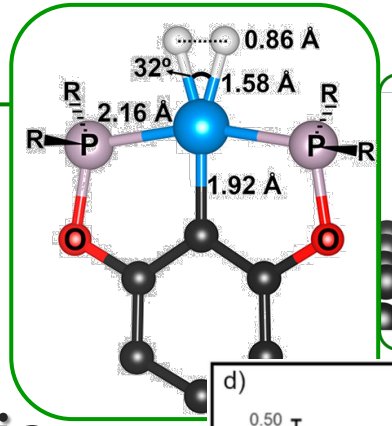
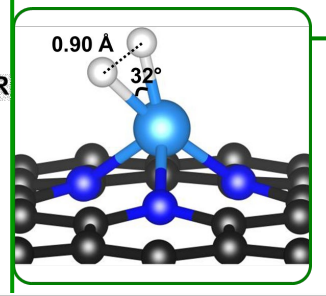
Conclusion

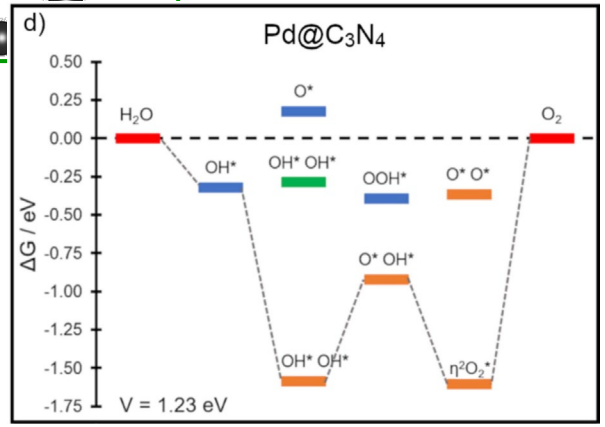


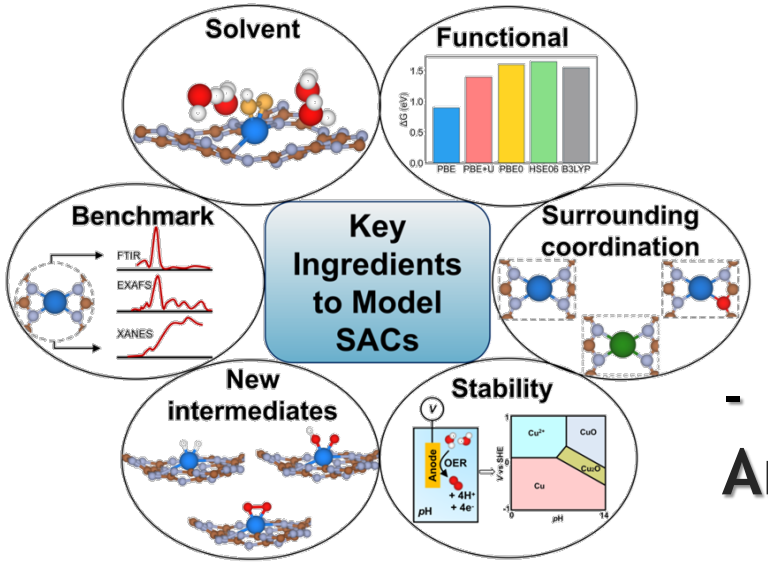




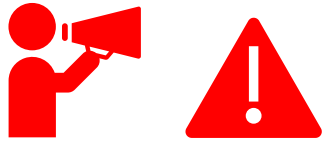
- Modeling of SAAs requires (at least) a few Ingredients

- SAAs are a viable way to reach new generation catalytic system





The chemistry and reactivity of SAAs is not easy



- SAAs are a fantastic playground to interplay experiments And theory

Thank you for your kind attention!

Gianvito Vilé,
Politecnico Milano

Fabio La Mantia,
University of Bremen

In-Hwan Lee, Korea University

Michail Stamatakis,
Oxford University

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