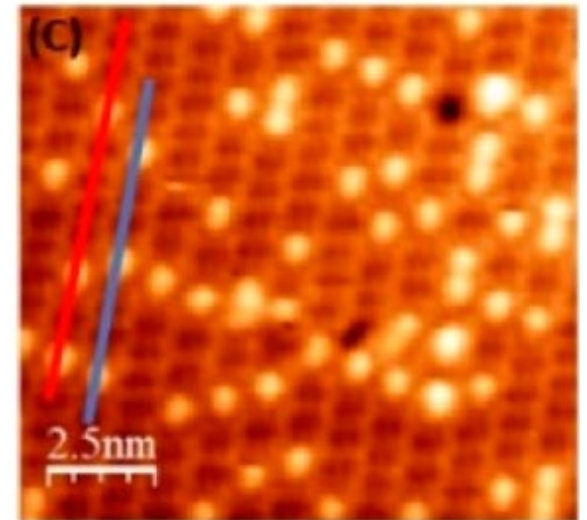
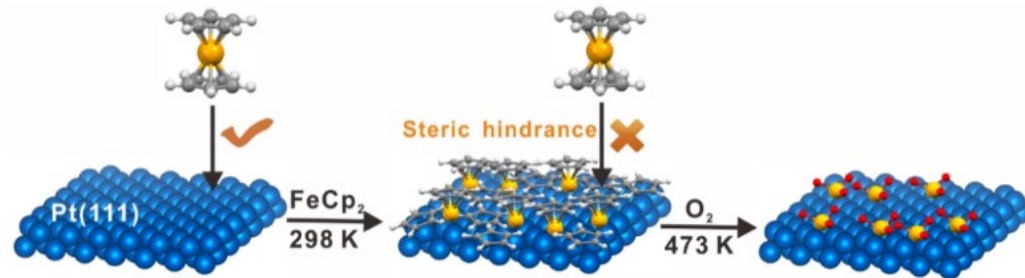
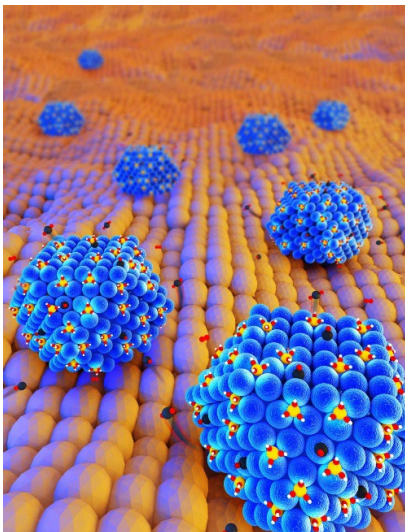


# Single Atom Catalysts for Sustainable Conversion of Synthetic Chemicals

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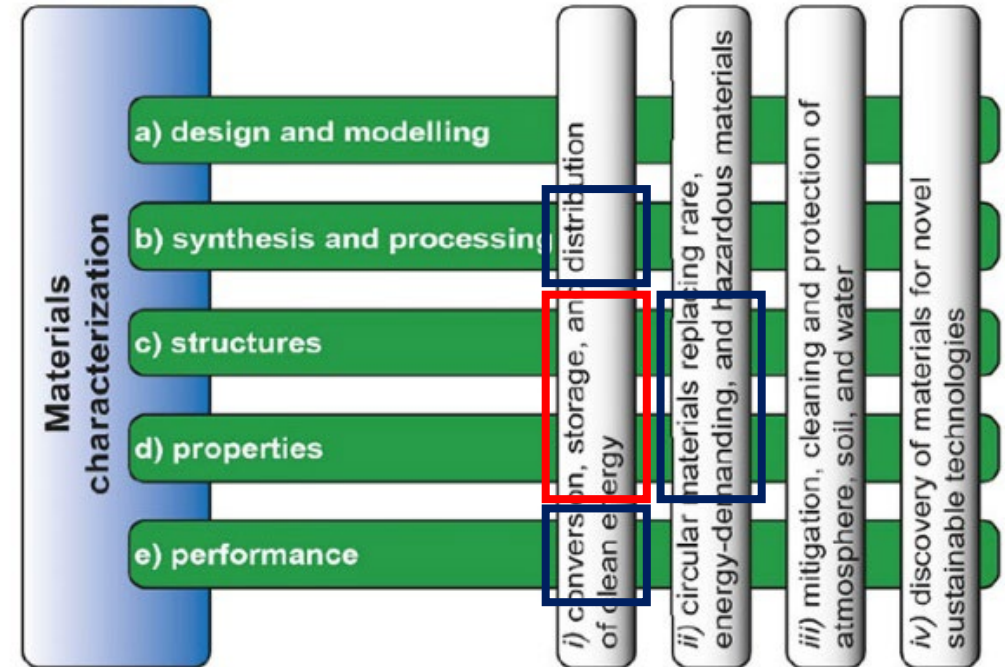
Storage from intermittent sources of power.

Heavy long-distance travel.

Transfer of energy between regions.

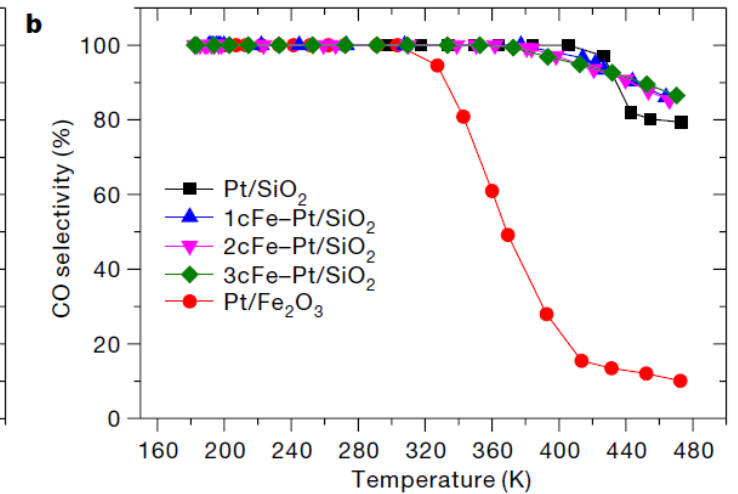
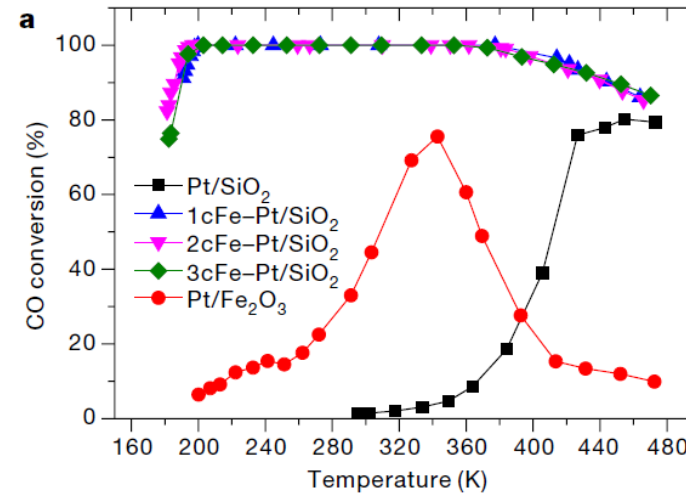
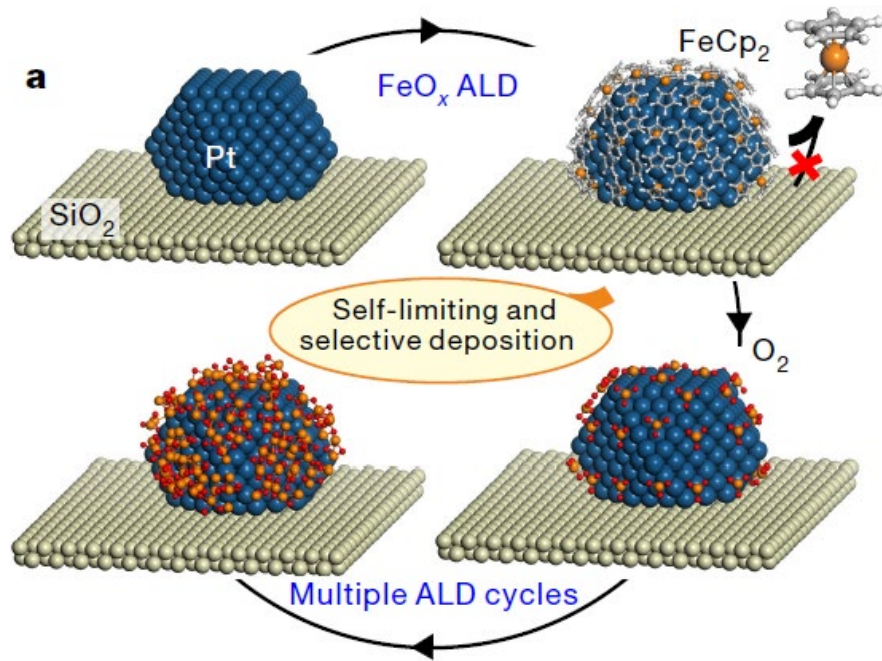
Chemical industry - 10% of Europe's consumption of fossil resources.

Energy dependence.



## Atomically dispersed iron hydroxide anchored on Pt for preferential oxidation of CO in H<sub>2</sub>

PROX reaction: 1% CO + 0.5% O<sub>2</sub> + 48% H<sub>2</sub> + He (balance)



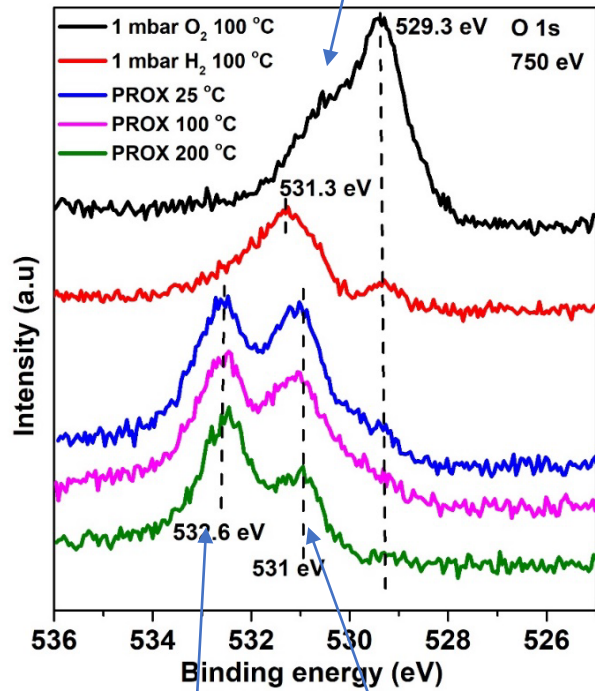
Cao L, Liu W, Luo Q, Yin R, Wang B, Weissenrieder J, et al. Atomically dispersed iron hydroxide anchored on Pt for preferential oxidation of CO in H<sub>2</sub>. *Nature* 2019 (7741) 631-5.

Chunlei Wang<sup>1</sup>, Heloise Tissot<sup>1</sup>, Markus Soldemo<sup>2</sup>, Junling Lu<sup>3</sup>, Jonas Weissenrieder, Inverse single-site Fe<sub>1</sub>(OH)<sub>x</sub>/Pt(111) model catalyst for preferential oxidation of CO in H<sub>2</sub>, *Nano Research* 15 (2022) 709-715

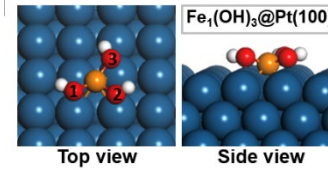
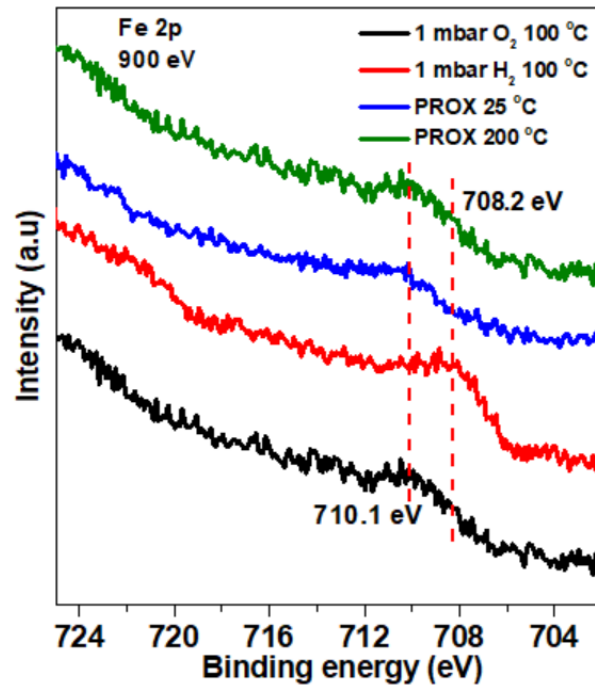
Ferrocene (FeCp<sub>2</sub>), steric hindrance, isolated sites

# In situ studies of 1c-Fe on Pt(111)

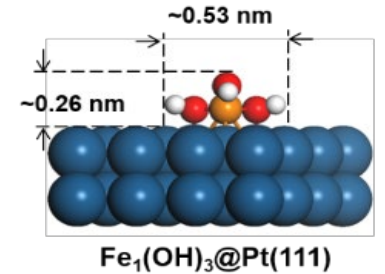
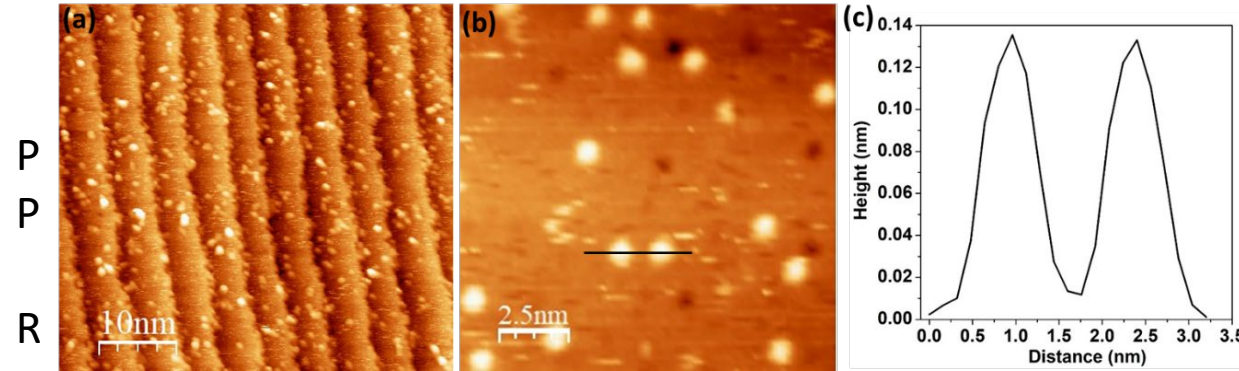
Hydroxylation



CO atop and bridge on Pt(111)

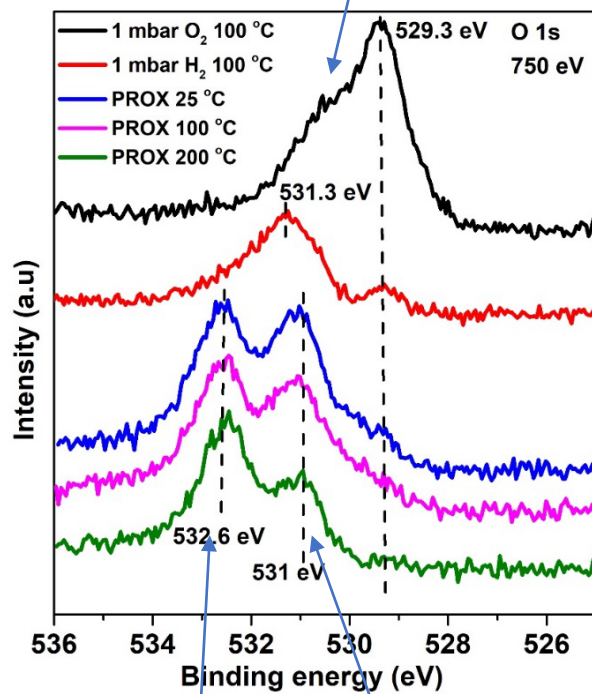


Fe <sub>1</sub> (OH) <sub>3</sub> @Pt(100)	Binding energy (eV)
1-OH	531.30
2-OH	531.21
3-OH	531.29

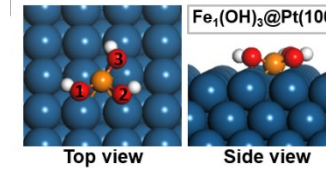
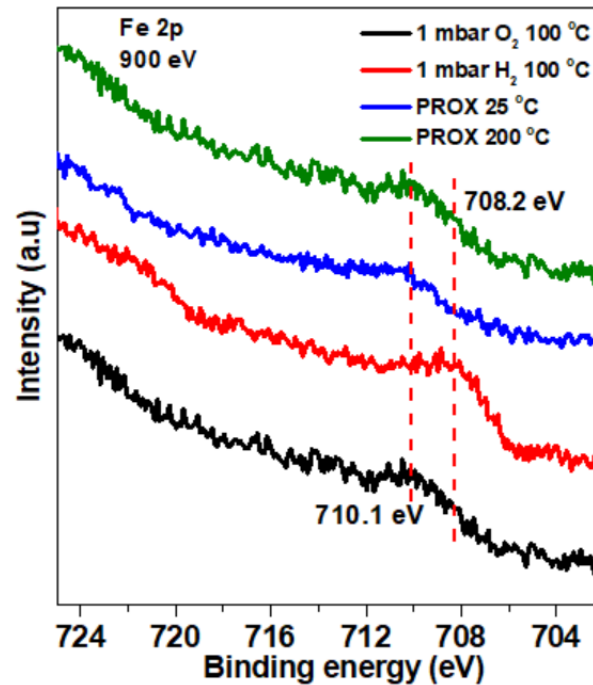


Reducible to Fe<sup>2+</sup>. Formation of a Fe(OH)<sub>3</sub> under PROX conditions

## Hydroxylation



CO atop and bridge on Pt(111)



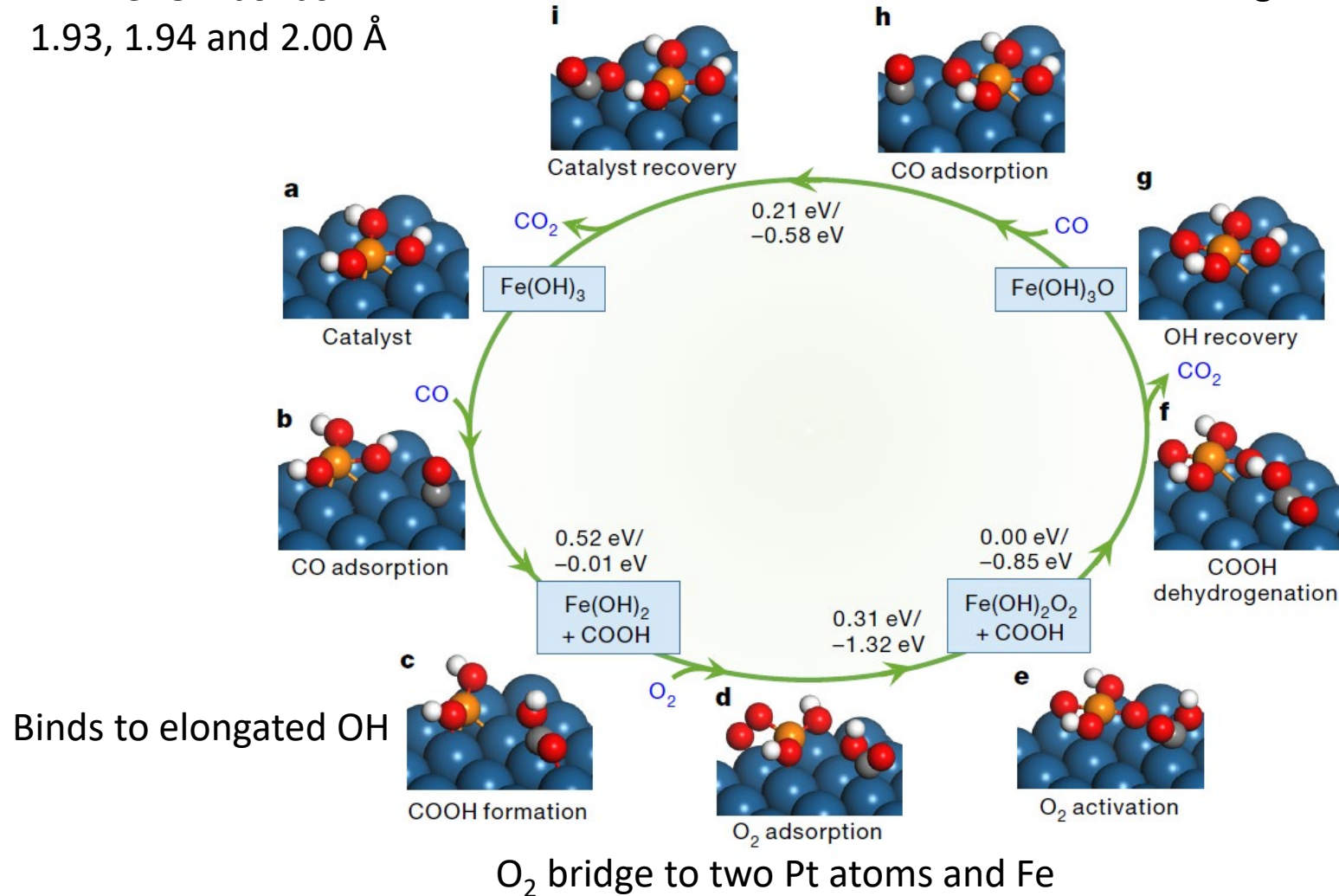
Fe <sub>3</sub> (OH) <sub>3</sub> @Pt(100)	Binding energy (eV)
1-OH	531.30
2-OH	531.21
3-OH	531.29



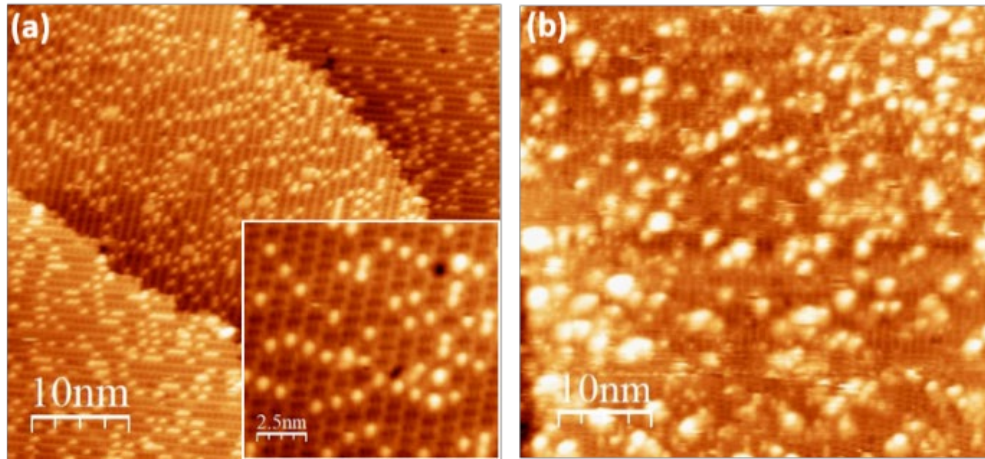
# Reaction pathway for CO oxidation during PROX

DFT Fe–OH bonds:  
1.93, 1.94 and 2.00 Å

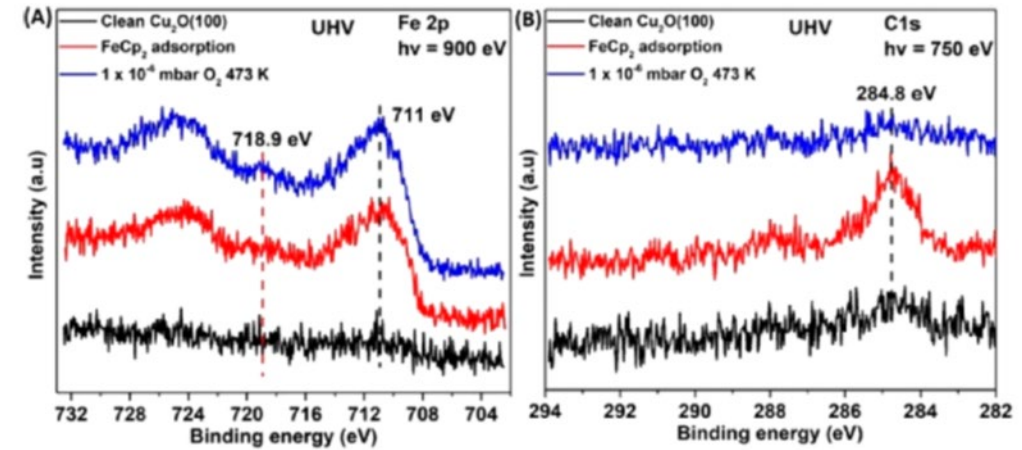
Binds to elongated O-



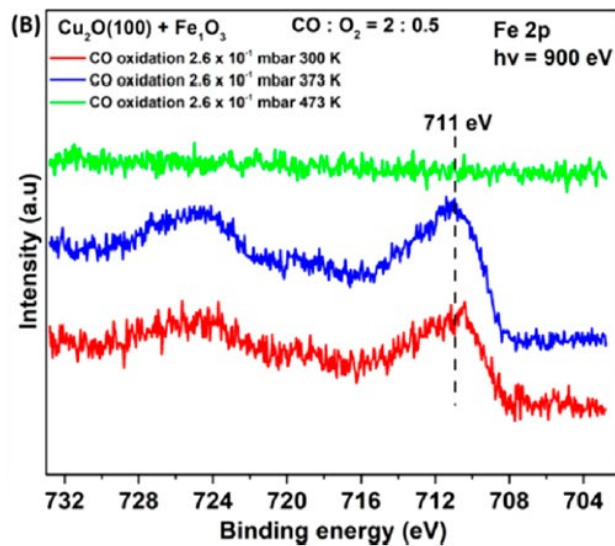
Fe(OH)<sub>3</sub> and Pt collaborate



STM of catalyst preparation



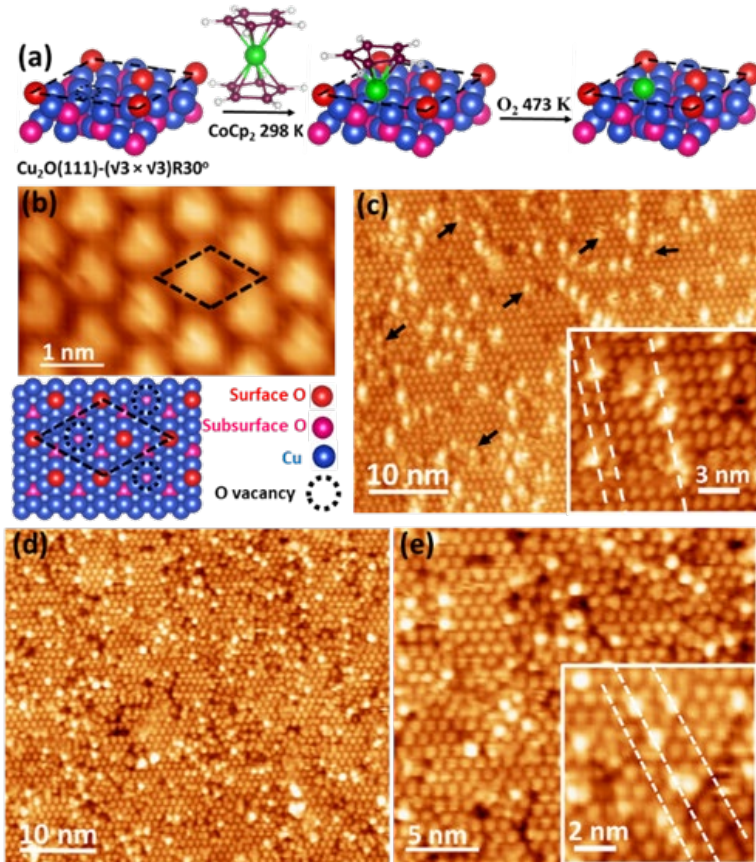
APXPS (MAX IV) of catalyst preparation



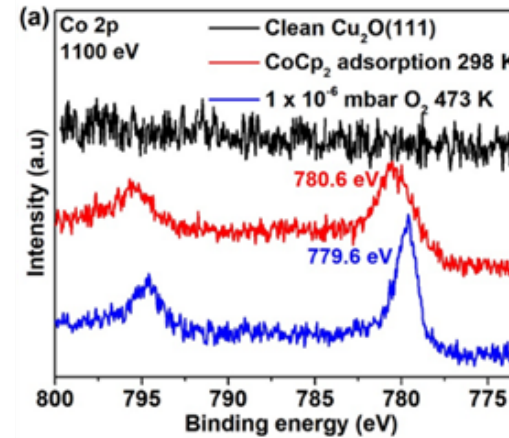
High-Density Isolated Fe<sub>1</sub>O<sub>3</sub> Sites on a Single-Crystal Cu<sub>2</sub>O(100) Surface  
 Chunlei Wang, Heloise Tissot, Joakim Halldin Stenlid, Sarp Kaya, and Jonas Weissenrieder  
 J. Phys. Chem. Lett. 2019, 10, 23, 7318–7323

Formation of stable isolated Fe centers

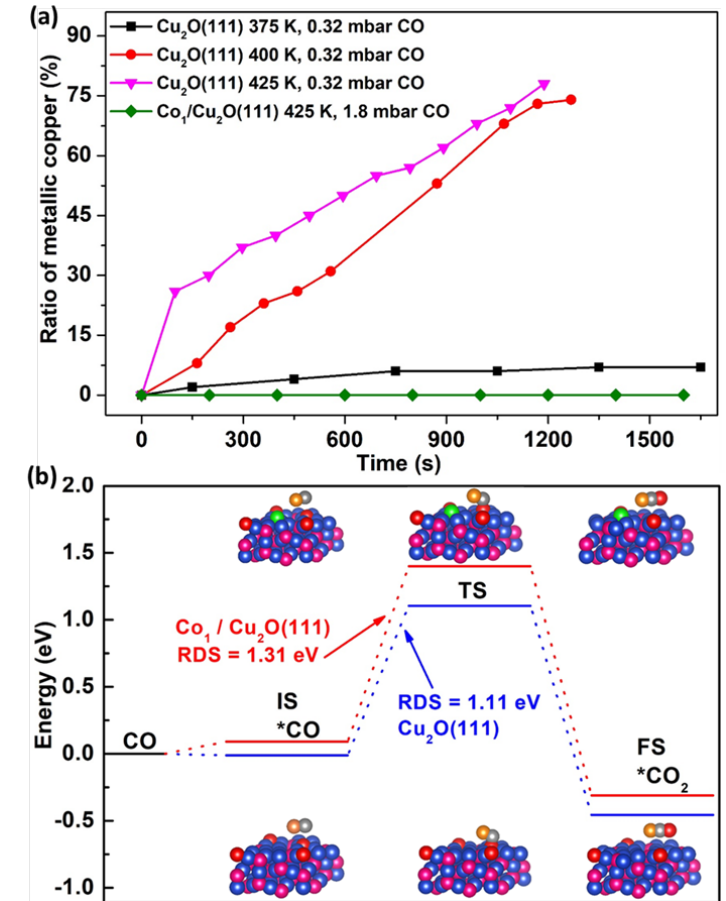
# Selective ALD deposition of Co on Cu<sub>2</sub>O(111) results in formation of isolated Co<sub>1</sub>Cu centers



STM of catalyst preparation



Co 2p (MAX IV)



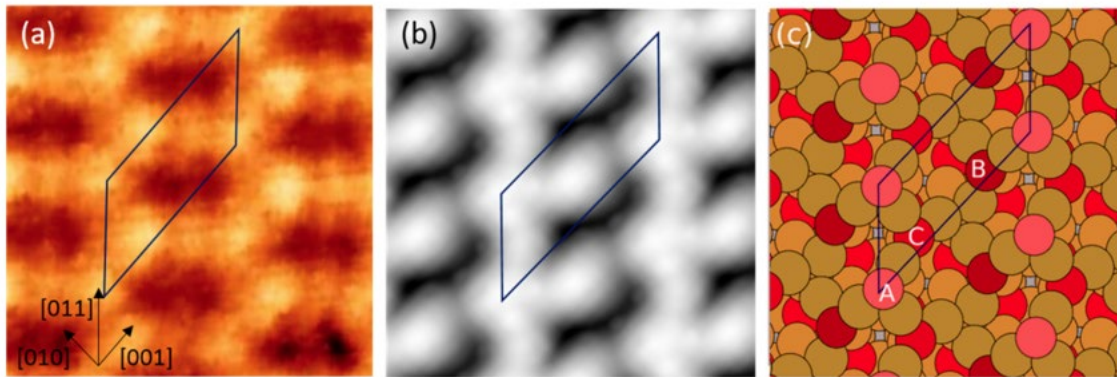
APXPS (MAX IV) and simulated reaction pathways

Stabilization of reactive Cu<sup>+</sup> sites .

Stabilization of Cu<sub>2</sub>O through Site-Selective Formation of a Co<sub>1</sub>Cu Hybrid Single-Atom Catalyst  
 C Wang, Y Kong, M Soldemo, Z Wu, H Tissot, B Karagoz, K Marks, et al,  
 Chemistry of Materials 34 (2022) 2313-2320



## In-Cu mixed oxides for CO<sub>2</sub> conversion



Cu<sub>2</sub>O(110) surface structure

ALD precursors

Copper dimers at the Cu<sub>2</sub>O(110) surface

Cu<sup>+</sup> sites

Structure, stability, chemical properties

Link to application portal: <https://kth.varbi.com/en/what:job/jobID:588420/where:4/>