



# Recent Research in Chen Group



## Development of novel catalysts in heterogeneous catalysis and electrocatalysis

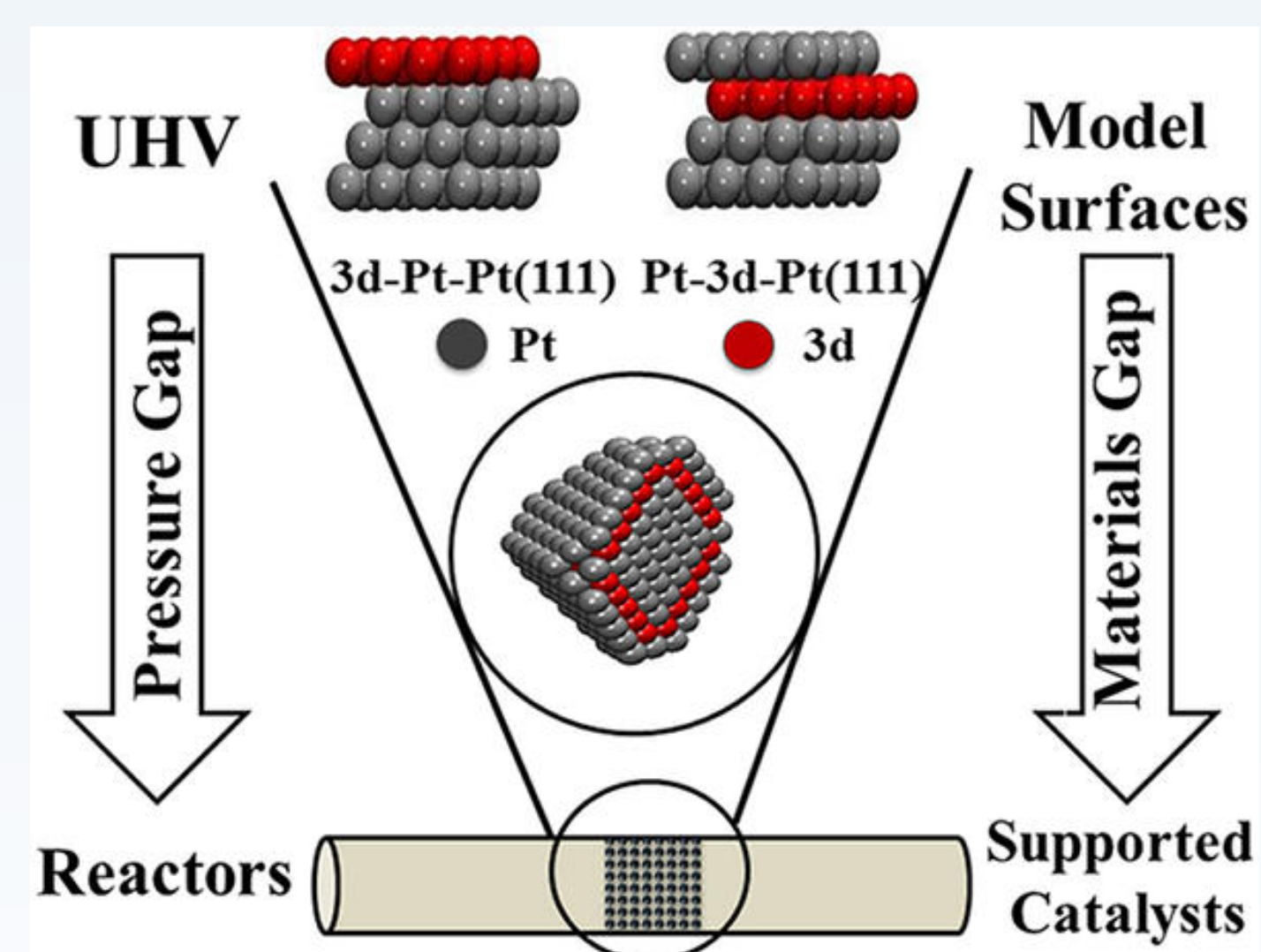
### Single crystal surfaces:

- Fundamental atomic-level understanding through experiments and theory

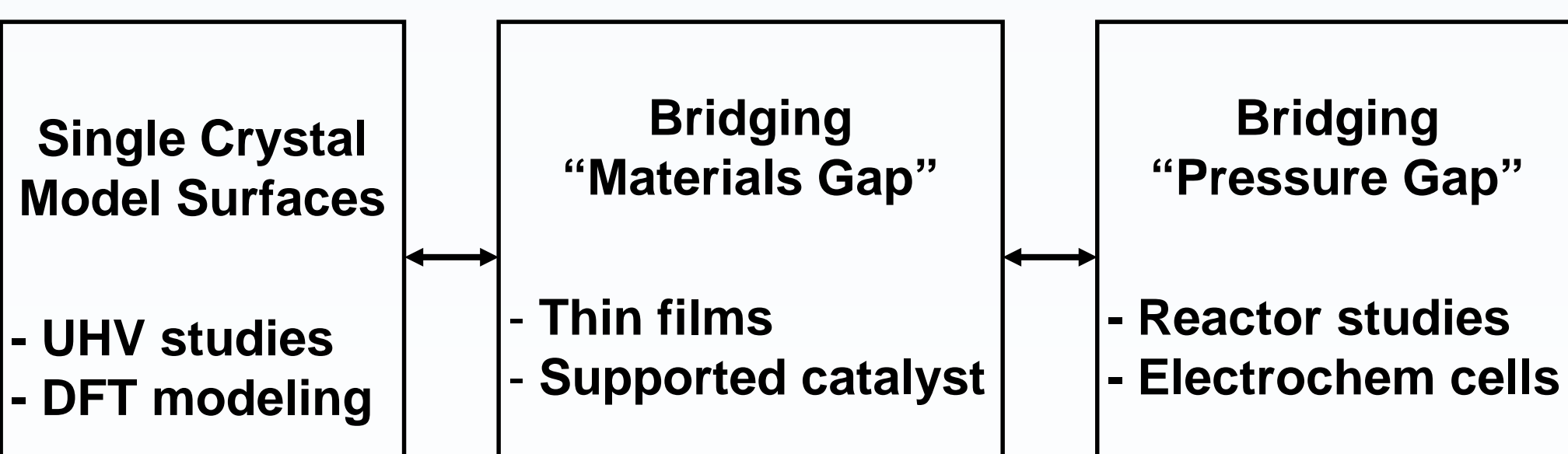
### Supported catalysts:

- More relevant to industrial catalysts and commercial processes

## Research approach: Combining model surfaces with supported catalysts



W. Yu, M.D. Porosoff, J. G. Chen, *Chemical Reviews* (2012).

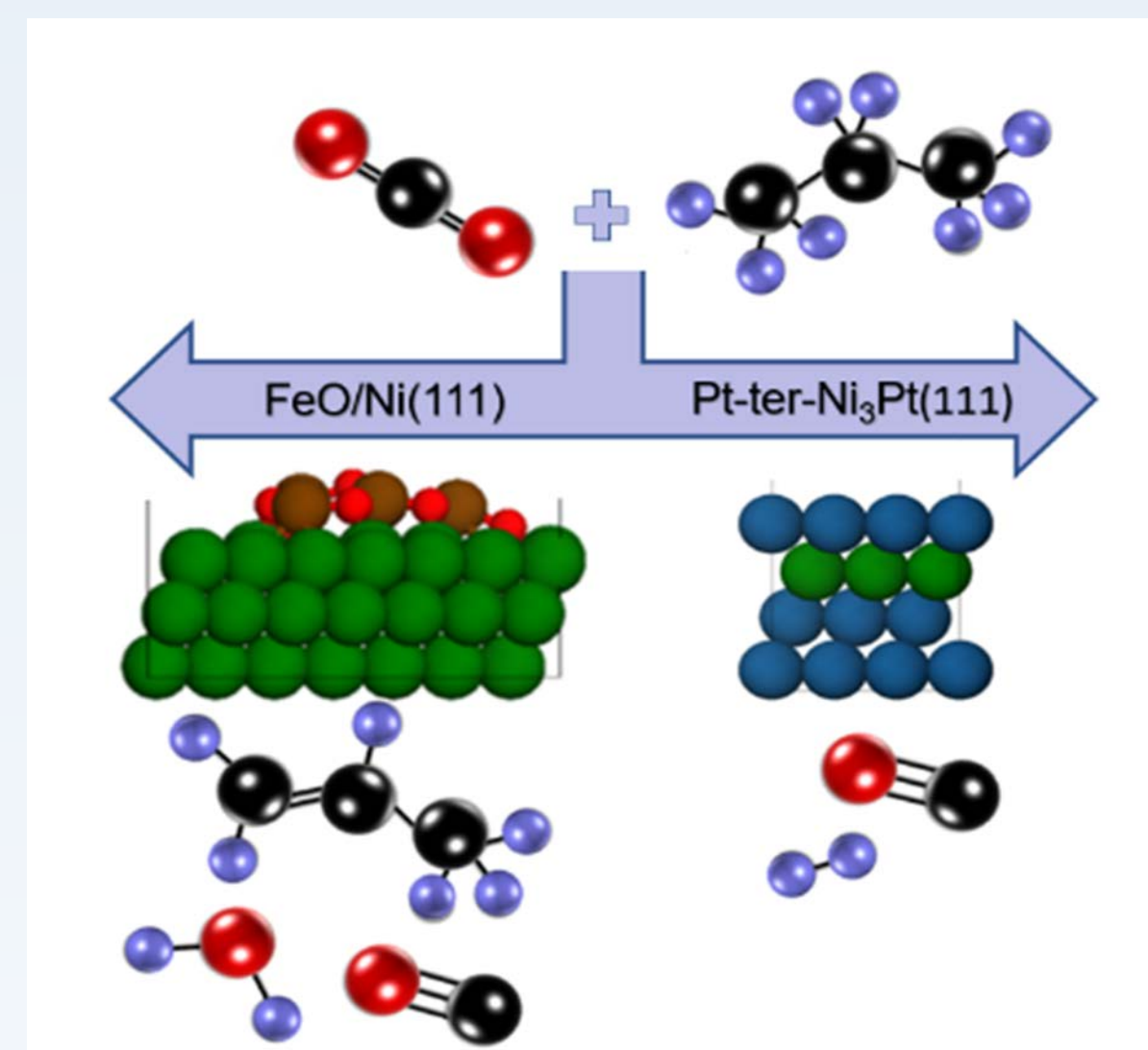
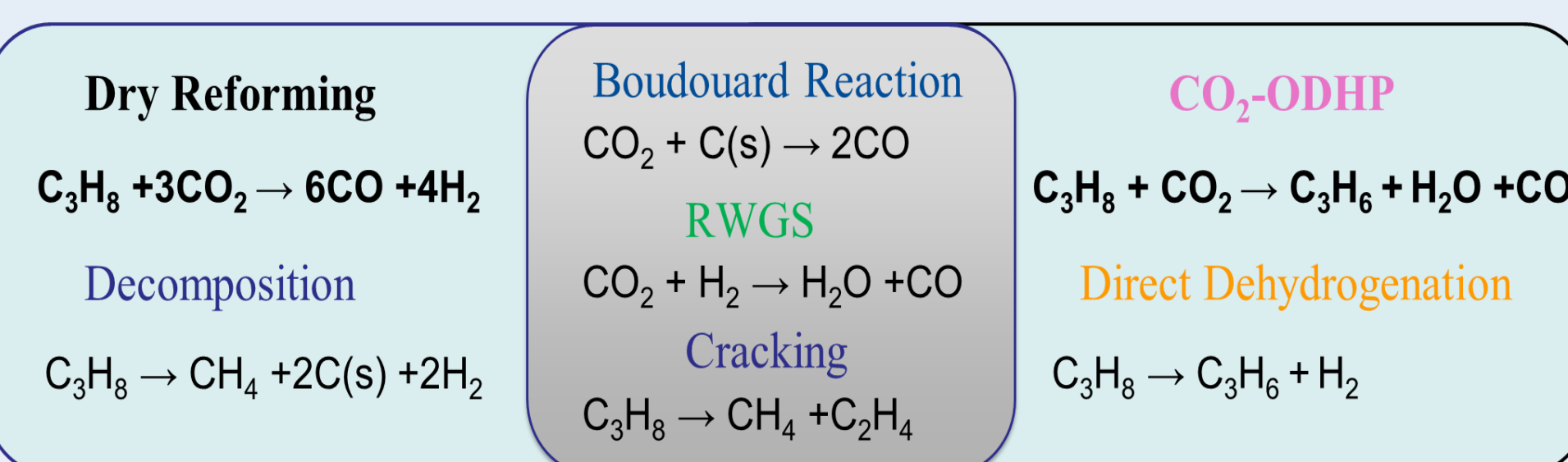


Bimetallic and carbide catalysts offer the advantages of reduced cost and enhanced activity, selectivity and stability.

## Example 1: Heterogeneous catalysis for CO<sub>2</sub> activation

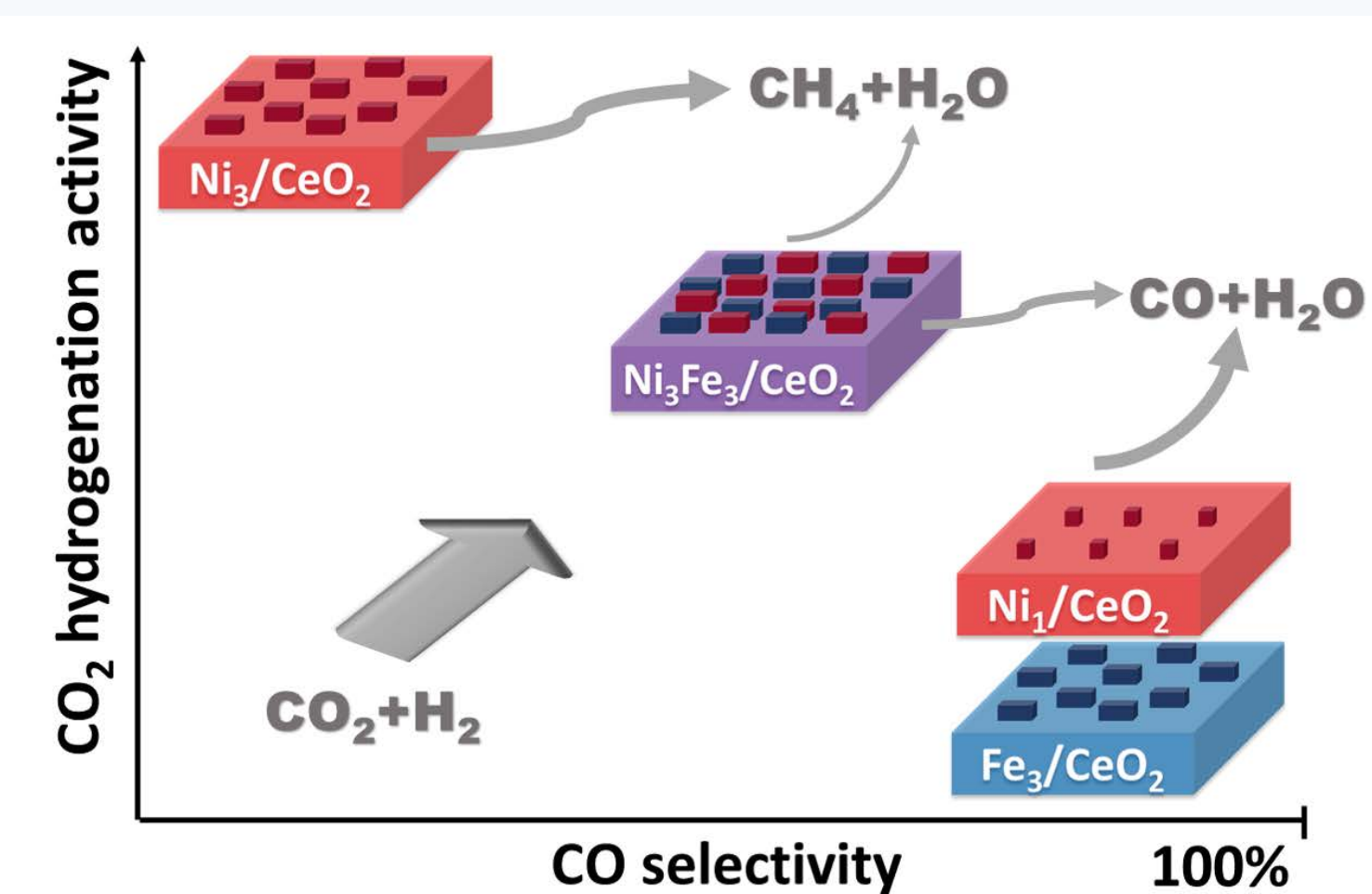
### Key reaction pathways:

- CO<sub>2</sub> reduction by light alkanes



E. Gomez, S. Kattel, B. Yan, S. Yao, P. Liu, J.G. Chen, *Nature Communications* (2018).

## Tuning selectivity with non-precious metal catalysts



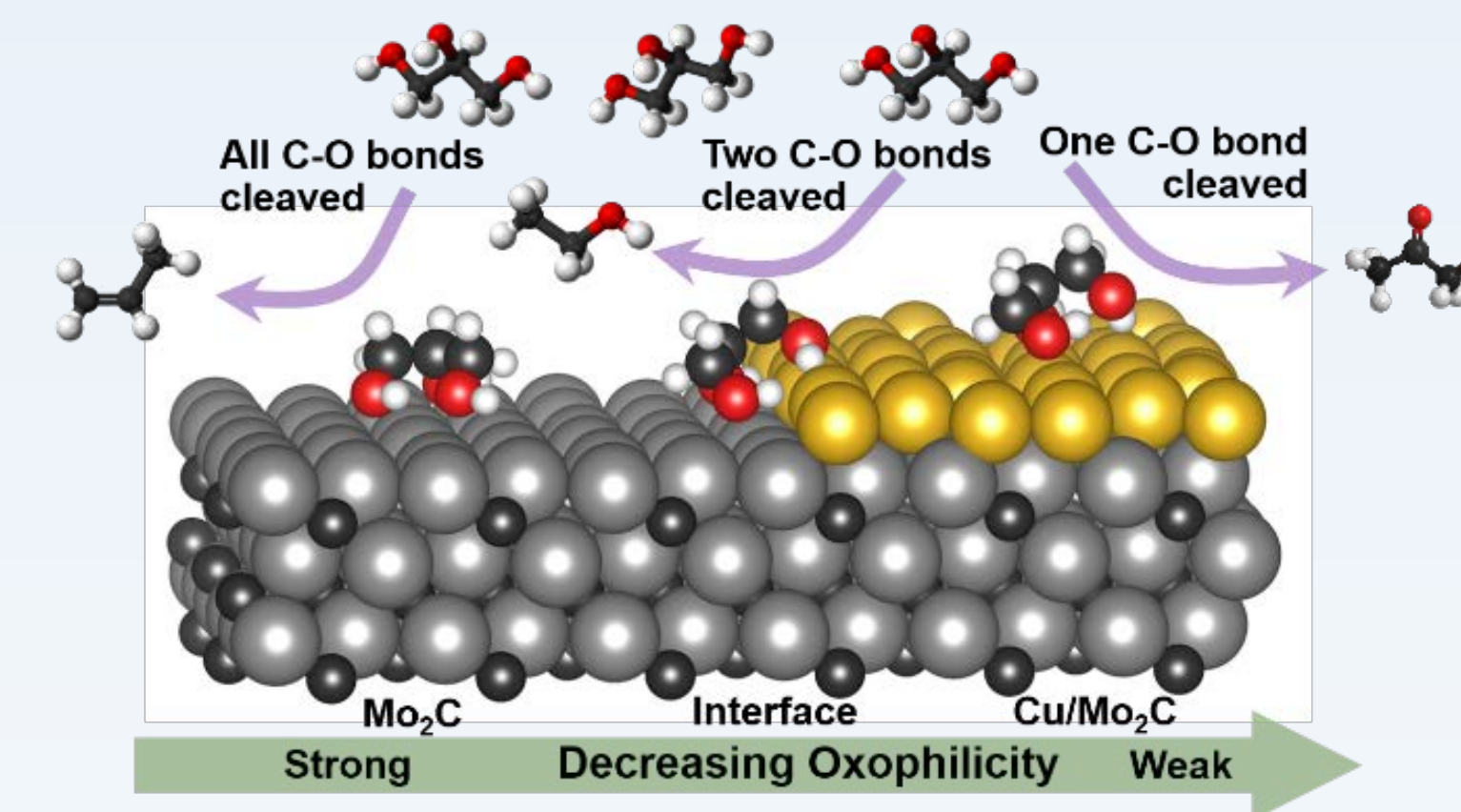
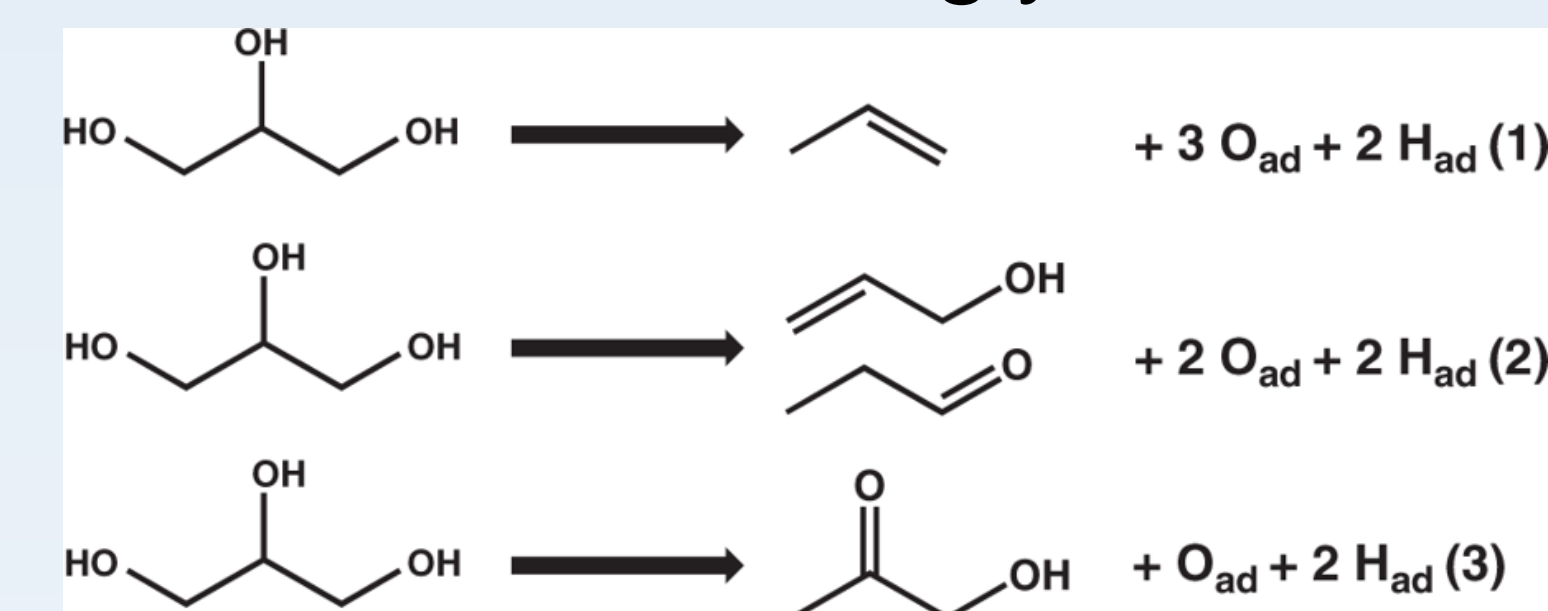
- Fe modification of Ni catalysts improves CO selectivity while maintaining high catalytic activity
- In-situ X-ray spectroscopy probes the phase and function of bimetallic catalysts

L.R. Winter, E. Gomez, B. Yan, S. Yao, J.G. Chen, *Applied Catalysis B: Environmental* (2018).

## Example 2: Conversion of inexpensive molecules into valuable chemicals

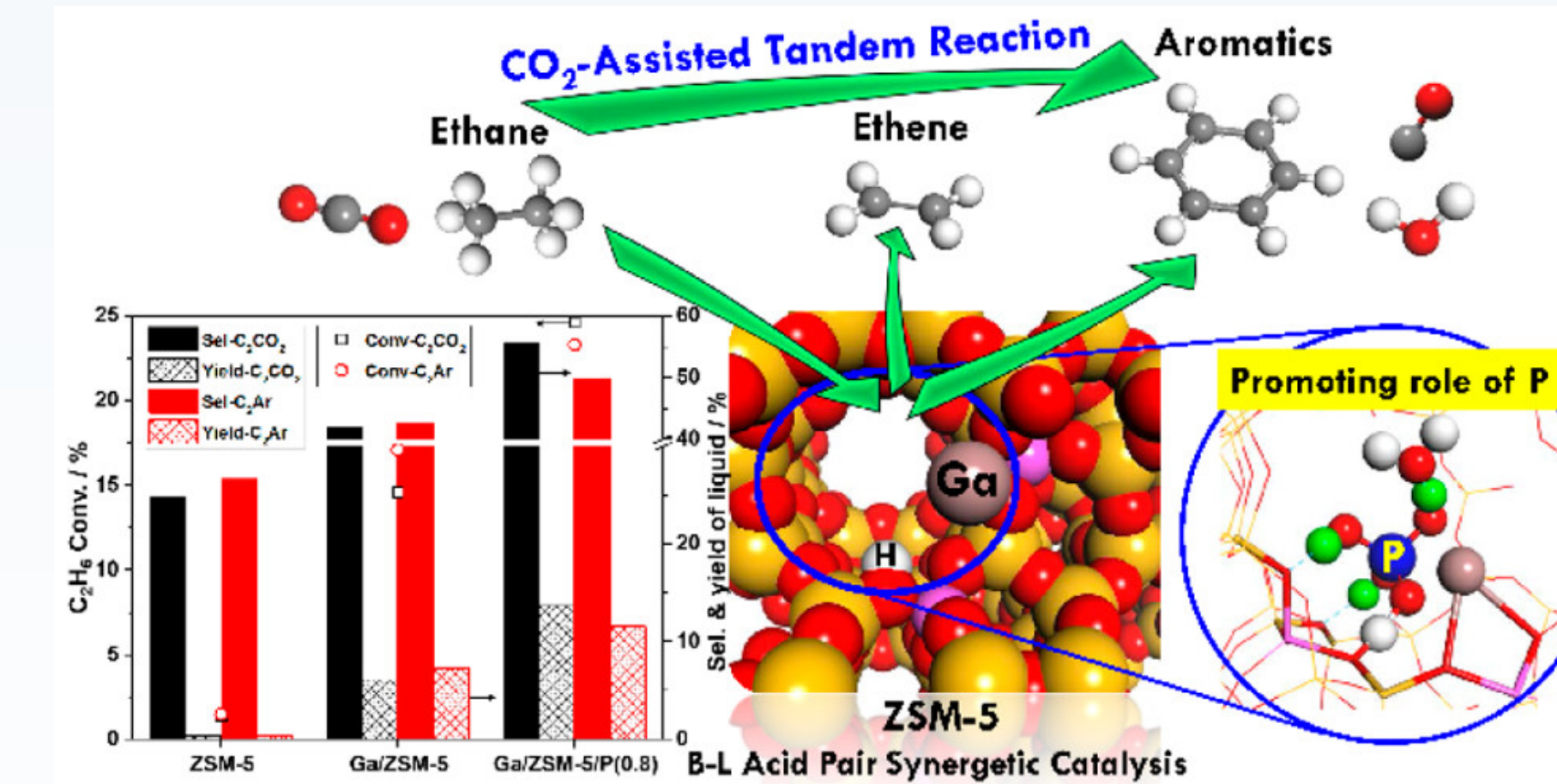
### Key reaction steps:

- Selective scission of C-O bonds in the HDO reaction of glycerol



W. Wan, S. Ammal, Z. Lin, K. You, A. Heyden, J.G. Chen, *Nature Communications* (2018).

## Tandem reactions of CO<sub>2</sub> reduction and ethane aromatization



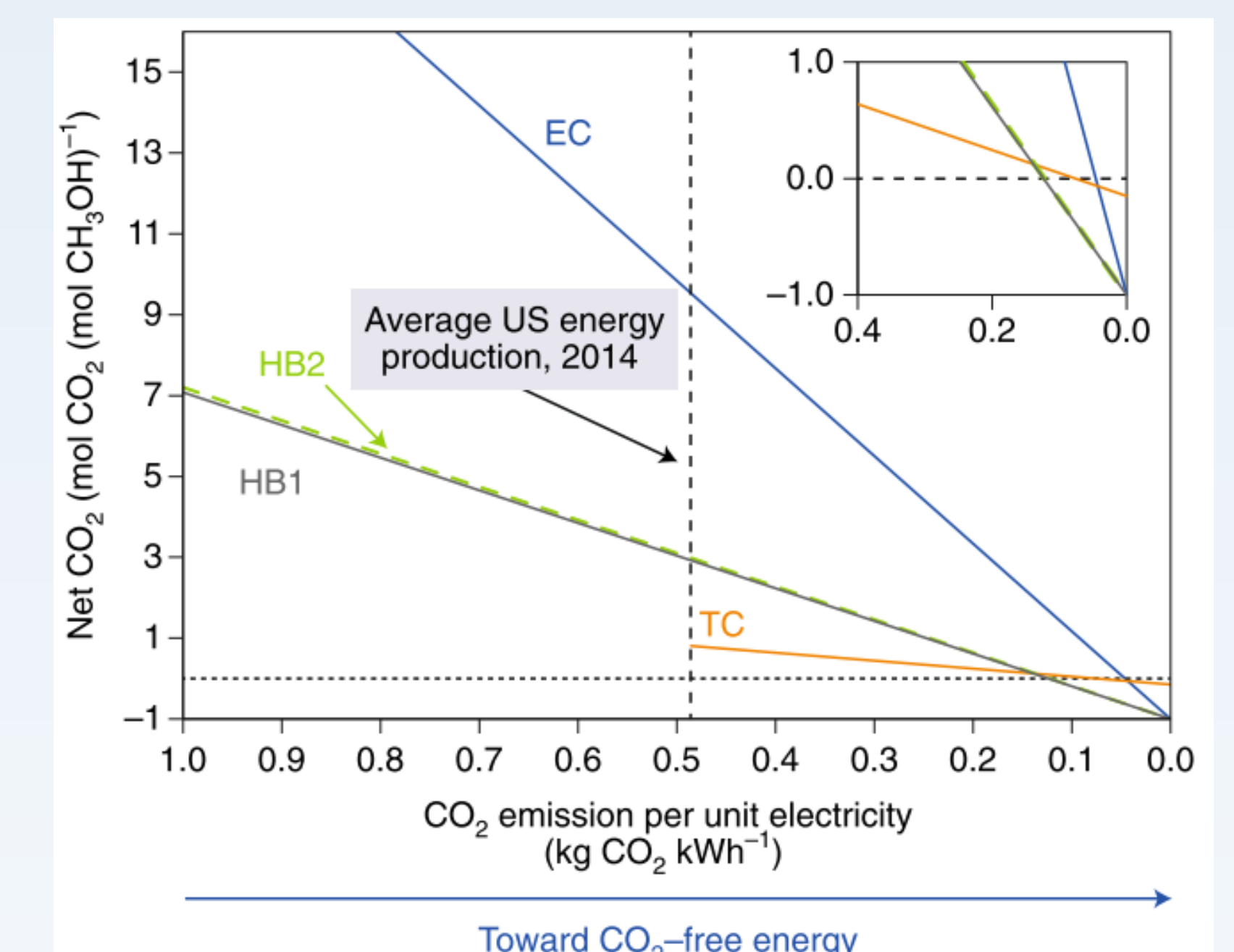
- Phosphorus (P)- and gallium (Ga)-modified ZSM-5 catalyzes a one-step reaction from CO<sub>2</sub> and ethane to aromatics
- DFT calculations provide insight into the effect of Ga- and P- modification, and the role of CO<sub>2</sub>.

E. Gomez, X. Nie, J.H. Lee, Z. Xie and J.G. Chen, *Journal of the American Chemical Society* (2019).

## Example 3: Electrocatalysis of CO<sub>2</sub> to value-added products

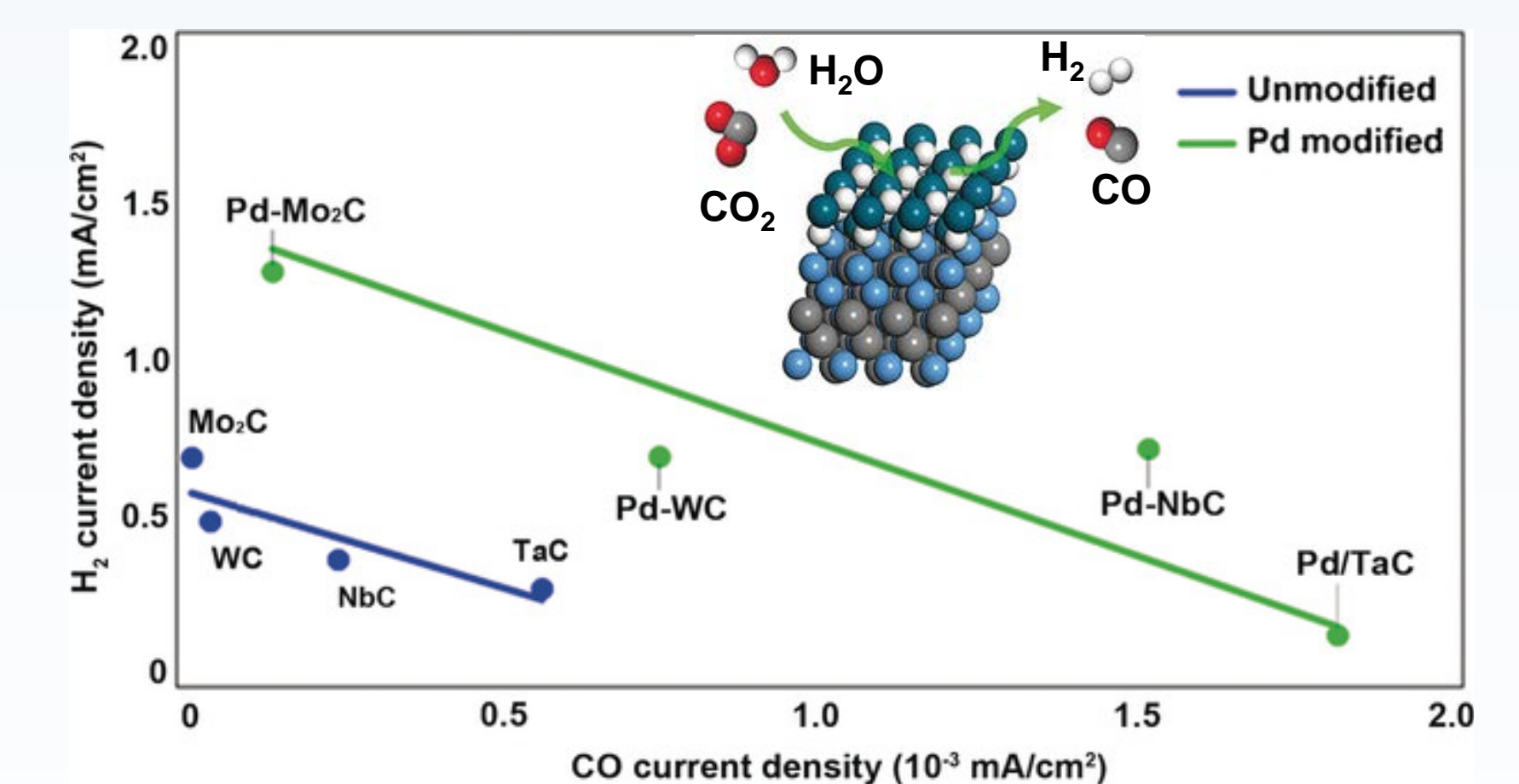
### Key reaction processes:

- Electrocatalytic (EC), thermocatalytic (TC), and combined hybrid (HB) processes for CO<sub>2</sub> reduction to methanol



B.M. Tackett, E. Gomez, J.G. Chen, *Nature Catalysis* (2019).

## Enhancing Activity and Reducing Cost for CO<sub>2</sub> Electrochemical Reduction



- Pd supported on transition metal carbides (TMCs) show high activity for the CO<sub>2</sub> reduction reaction to produce syngas (CO/H<sub>2</sub> mixture)
- By supporting Pd on TMCs, the cost of the catalyst can be reduced

J. Wang, S. Kattel, C.J. Hawhurst, J.H. Lee, B.M. Tackett, K. Chang, N. Rui, C.-J. Liu and J.G. Chen, *Angewandte Chemie International Edition* (2019).