

# PROJECT 30: INNOVATIVE PROCESS FOR CO<sub>2</sub> CONVERSION TO HIGH ADDED VALUE CHEMICALS AND FUELS BASED ON HYBRID CATALYSTS

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Research Centre  
for Gas Innovation

cleaner energy for a sustainable future

Workshop RCGI  
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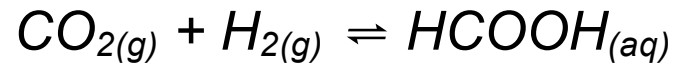
# OBJECTIVES

*The major goal of this project is the development catalytic processes using hybrid catalysts for the conversion of CO<sub>2</sub> into high added value chemicals and fuels.*

*High added value chemicals and fuels production via innovative CO<sub>2</sub>-to-liquid processes, including **nanotechnology and bioinspired approaches**, to achieve optimized processes at mild conditions and high selectivity compared to traditional implemented processes.*

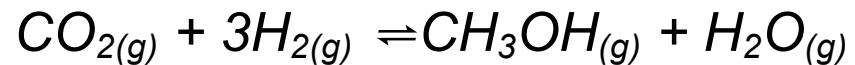
## CO<sub>2</sub> Hydrogenation

Hydrogenation to  
Formic acid

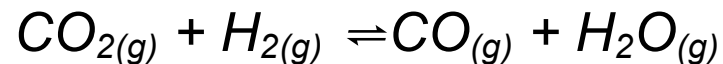


(Typical product in homogeneous catalysis)

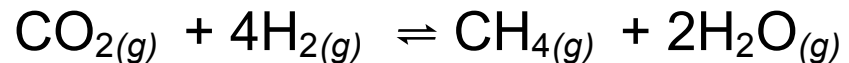
Hydrogenation to  
methanol



Reverse water-gas  
shift (RWGS)



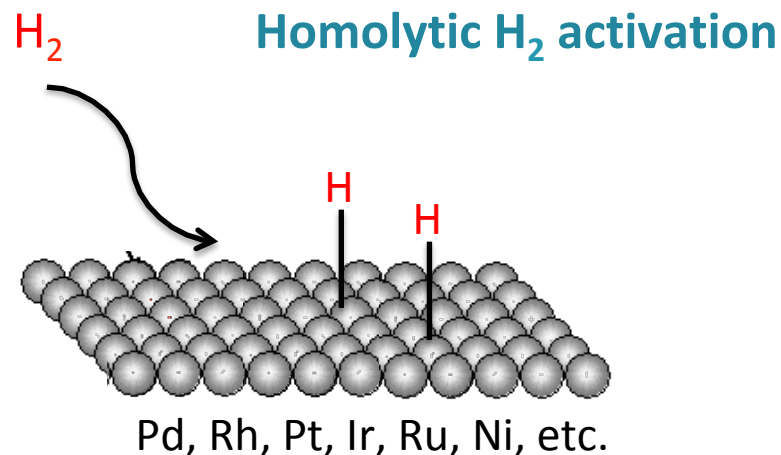
Methanation



✓ Hydrogenation to higher alcohols and olefins

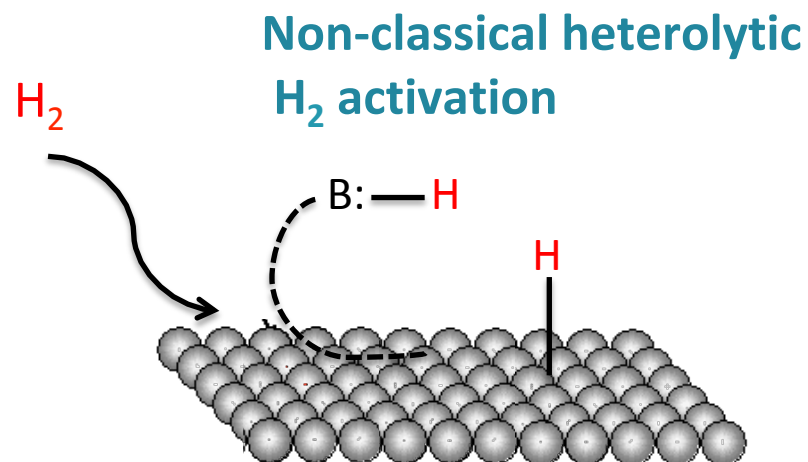
# *H<sub>2</sub> activation on metal surfaces*

## 1) Metals with favorable H<sub>2</sub> dissociation (usually barrierless)



## 2) Metals with unfavorable H<sub>2</sub> dissociation

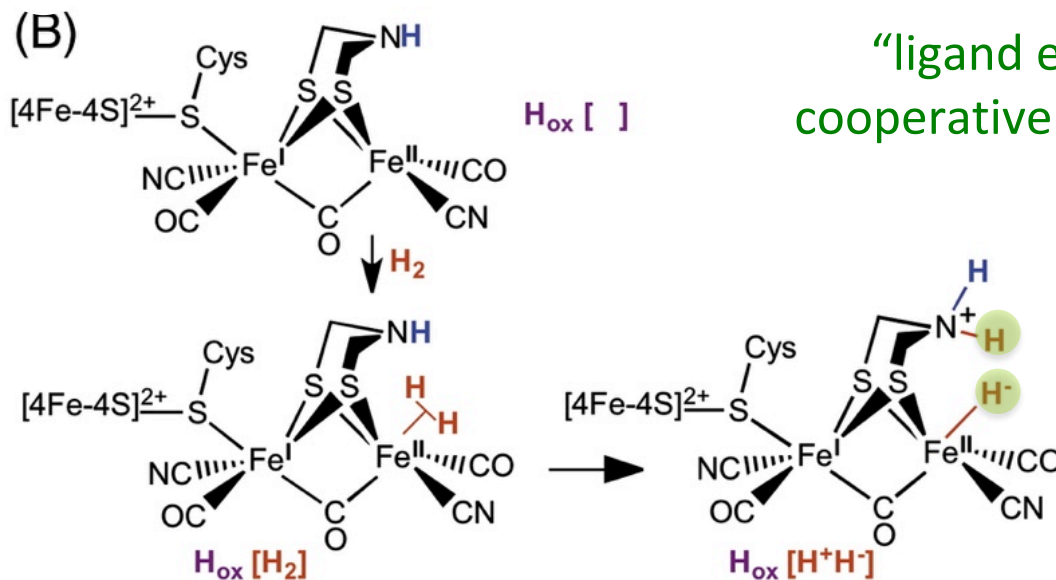
- Surface defects (size, shape)
- Light (plasmonic catalysis)
- Add a second metal (ex. Pd, Pt)
- Metal-support interface (Au/TiO<sub>2</sub>)
- **Metal-ligand interface (Au/L)**



# Non-classical heterolytic splitting of $H_2$

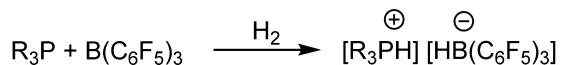
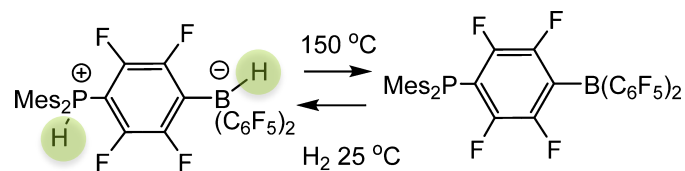
@ enzyme catalysis

FeFe-hydrogenase

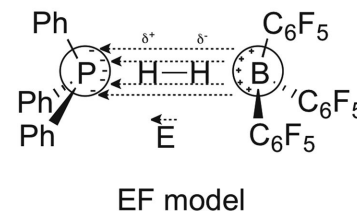
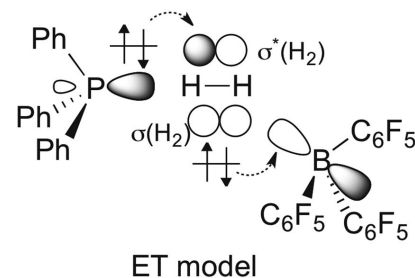


# Non-classical heterolytic splitting of $H_2$

## @ main-group frustrated Lewis pairs (FLP)



“metal-free hydrogenation”

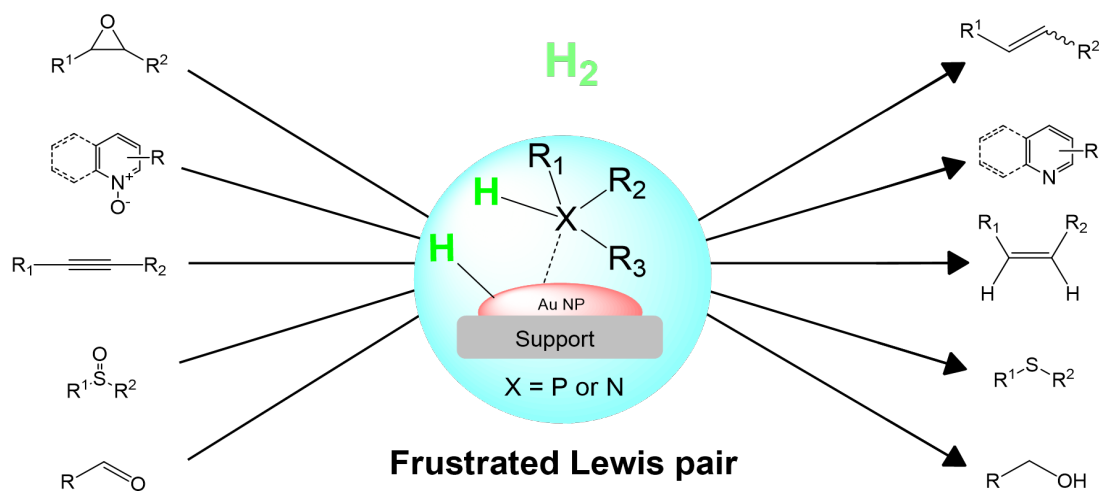


Stephan D.W. et al *Science* 314, 1124–1126 (2006)

Rokob, T. A. et al. *Angew. Chem., Int. Ed.* 47, 2435–2438 (2008).  
Grimme, S. et al. *Angew. Chem., Int. Ed.* 49, 1402–1405 (2010).

# Activation of H<sub>2</sub> via frustrated Lewis pairs

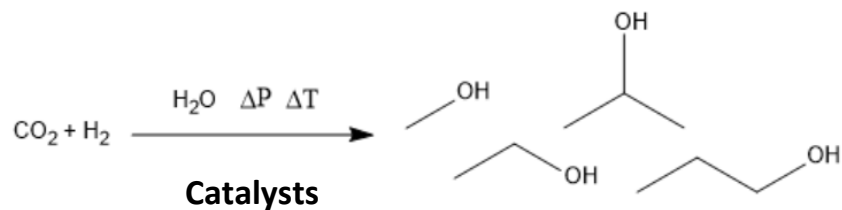
## Au@N-containing ligand Au@N-doped carbon FLP analogous



- Fiorio, J. L., R. V. Gonçalves, E. Teixeira-Neto, M. A. Ortuño, N. López and L. M. Rossi *ACS Catal.* **8**, 3516–3524 (2018)
- Patent: Fiorio, J. & Rossi, L. M. BR 10 2018 004902 0



# Direct Conversion of CO<sub>2</sub> to higher alcohols





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**THANK YOU**



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