catCHy

EUROPEAN TRAINING NETWORK

Novel catalysts for CO_2 Hydrogenation and Electro-reduction

PAUL SCHERRER INSTITUT PSI

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Mid-Term Review Meeting

Budapest (April 22, 2022)

About Me

- BTech in Chemical Engineering
  VIT, India
- MSc In Chemical Engineering
  TU Delft, Netherlands
- Started PhD on Oct. 1, 2021

- Supervised by:
  - Dr. Olga Safonova, PSI
  - Prof. Christophe Copéret, ETH Zurich

Role in CATCHY

WP2 — *In situ* XAS & IR Characterization

- Design cells for spectroscopy
- Implement characterization techniques for clusters deposited on *flat* substrates

WP5 — Exploring Novel Catalytic Systems

- Explore role of Ag in various systems
- Draw correlations with established systems
- Compare cluster systems

WP2: *In situ* XAS & IR Characterization of (Bi)metallic Clusters for Thermocatalysis

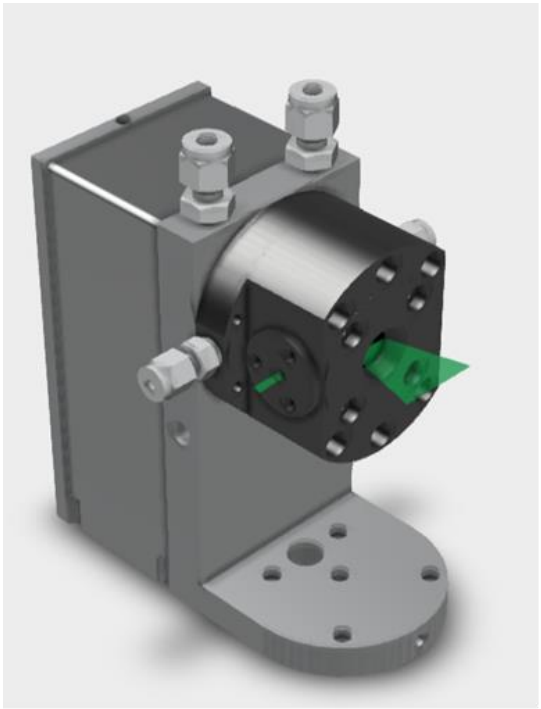
X-Ray Technique

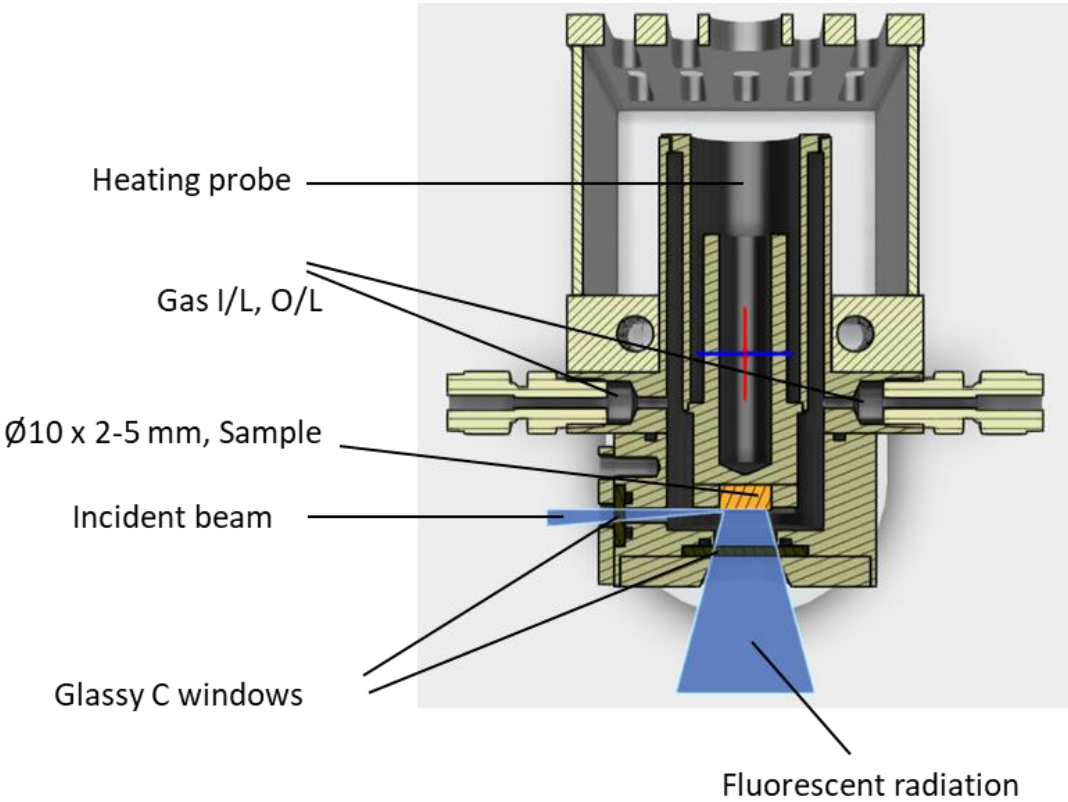
- Fluorescence Mode Absorption
  - ✓ Design *in situ* cell (grazing incidence) for clusters supported by *flat* substrates
  - ○ Fabricate cell and arrange analytics **(*May, '22*)**
  - ○ T-P stability test **(*June, '22*)**
  - ○ Proof-of-concept CO-adsorption on Pt clusters **(*March, '23*)**

IR Techniques

1. Polarization-Modulation Absorbance (PM-IRRAS)
   - ✓ Modified existing design for Brucker PMA50[1]
   - ✓ Fabricated prototype
   - ○ Analytics ,T-P stability test **(*June, '22*)**
   - ○ Proof-of-concept CO-adsorption on Pt clusters **(*August, '22*)**
2. Diffusive-Reflectance (DRIFTS)
   - ○ Proof-of-concept CO-adsorption on Pt clusters **(*July, '22*)**

1 = J. Chem. Phys., 124, 054717 (2006)





Novel XAS-Fluorescence Mode cell for *flat* support samples (Operable @25 bar, 300° C)

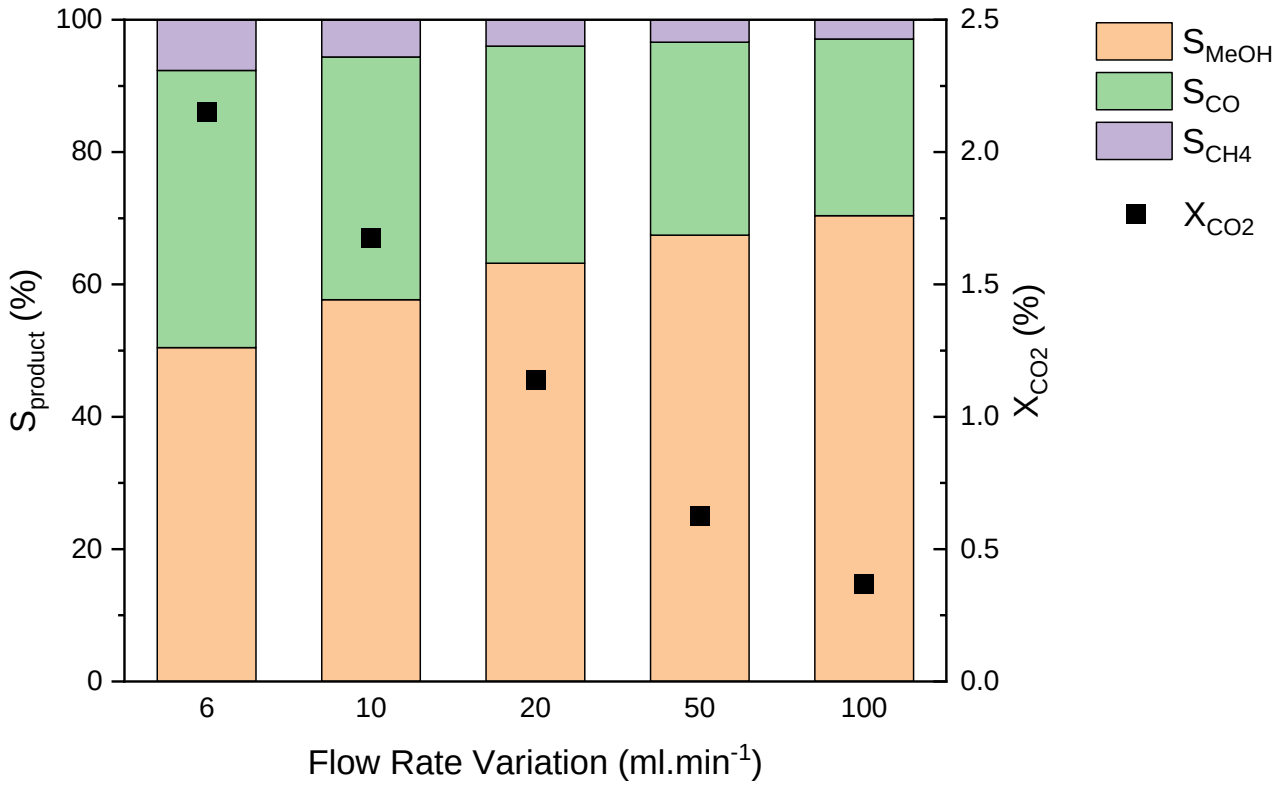
WP5: Exploring (Bi)Metallic Compositions for CO_2 Hydrogenation

Classical Impregnation Approach

- ✓ Ag-Zn/X powdered samples
  - Ag:Zn = 1:1 a.r. (10% total wt loading)
  - Testing at 250° C, 40 bar and varying flowrates
  - X = ZrO_2
    - Very low (<0.5 X_{CO2}) activity
  - X = SiO_2
    - Stable over 30 h TOS

- Ag-Zn/SiO_2 powdered samples ***(May, '22)***
  - Vary a.r. to explore particle size effects

- Ag-X/SiO_2 powdered samples ***(July, '22)***
  - X = Cu, Pd, Ni, Ga, …
  - Explore *bimetallic* chemical space



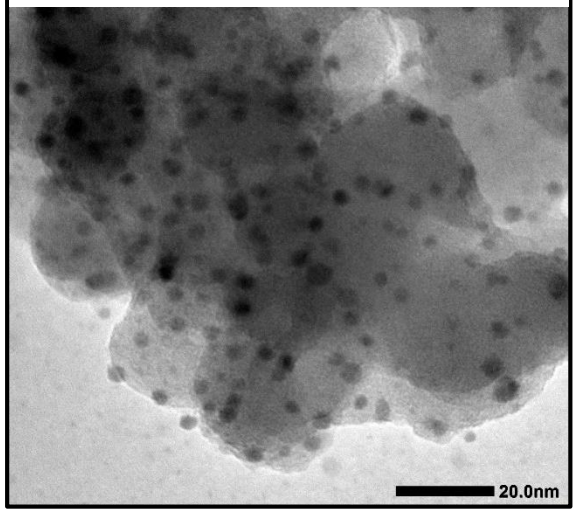
Ag-Zn/SiO_2 sample tested 4 MPa, 250° C, CO_2:H_2 = 1:3

WP5: Exploring (Bi)Metallic Compositions for CO_2 Hydrogenation

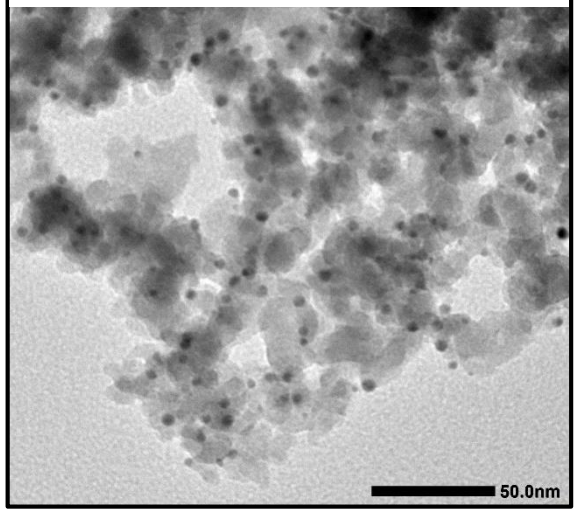
Surface-Organometallic Approach

- ✓ Powdered samples synthesized via SOMC
  - $Ag/SiO_{2\text{-}700}$ (0.3 wt%)[1]
  - $Ag_{0.8wt\%}\text{-}Zn_{0.12wt\%}/SiO_{2\text{-}700}$[1,2]
  - Very low activity (<0.1% X_{CO2})
    - Attributed to lower loading or specific a.r.
- ○ Reproduce "*successful*", classically impregnated systems

$Ag/SiO_{2\text{-}700}$ (3.4 nm ± 0.08 nm)



$Ag\text{-}Zn/SiO_{2\text{-}700}$ (3.98 nm ± 0.07 nm)



1 = JJ Corral-Pérez, C. Copéret, A. Urakawa, J. Catal., 380, **2019**, 153-160
2 = L. Rochlitz et al., Chem. Sci. J., **2020**, 11, 1549-1555

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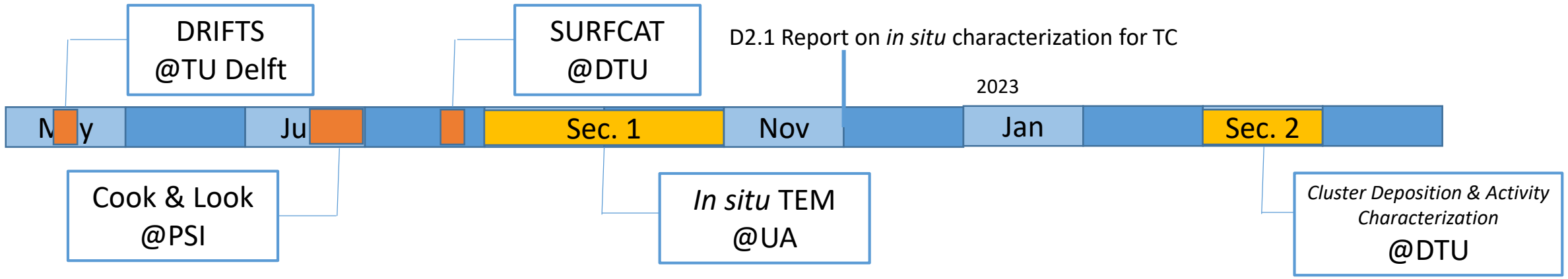

Thank you!