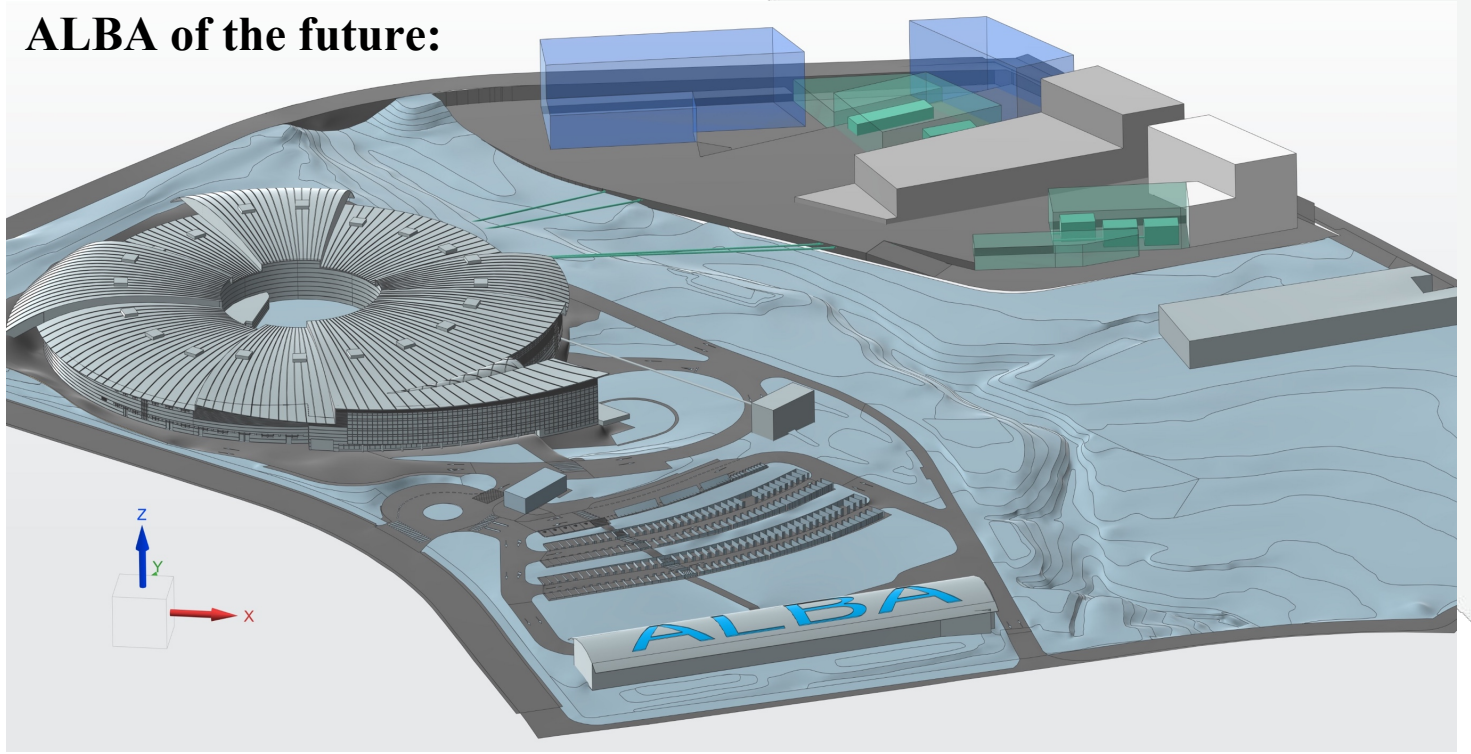


Past Scientific Outcomes and Future Directions at ALBA

Presented By : Ravi Ranjan

06th November 2024 – Postdoc Day

The Scientific Background:

Educational Background:

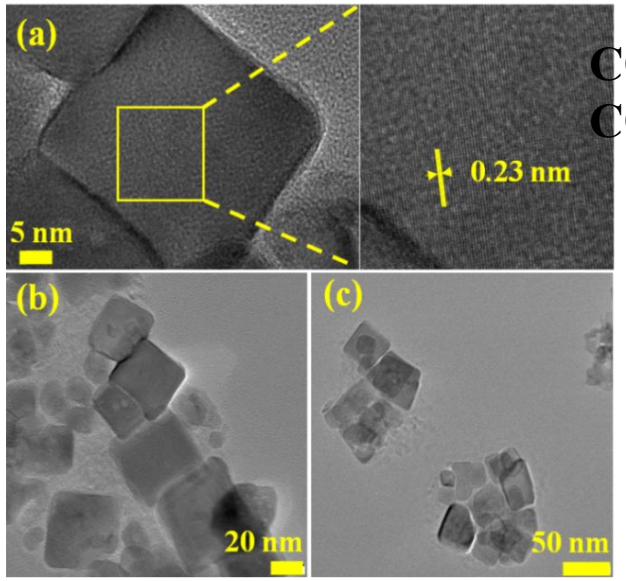
- **Thesis title and advisor:** "*Gas-Solid Interaction and its Influence in Electronic Structure Evolution and Heterogeneous Catalysis*" under the supervision of **Dr. C. S. Gopinath** at CSIR-NCL, Pune, India.

Scientific Interest:

- **Field(s):** Heterogeneous Catalysis and Surface science
- **Key achievements:**
  1. Authored and co-authored 11 research papers and 1 patent during my Ph.D. program
  2. Received the B.D. Kulkarni Award for the best research publication with the highest impact factor in Chemical Engineering/Technology in 2023 at CSIR-NCL, Pune
  3. Initial report on the high-temperature metal-insulator transition in the VO_2 phase of vanadium
  4. Initial report for CO_2 reduction in hydrogen lean condition to achieve 100 % CO selectivity
- **Key publications and Patents:**

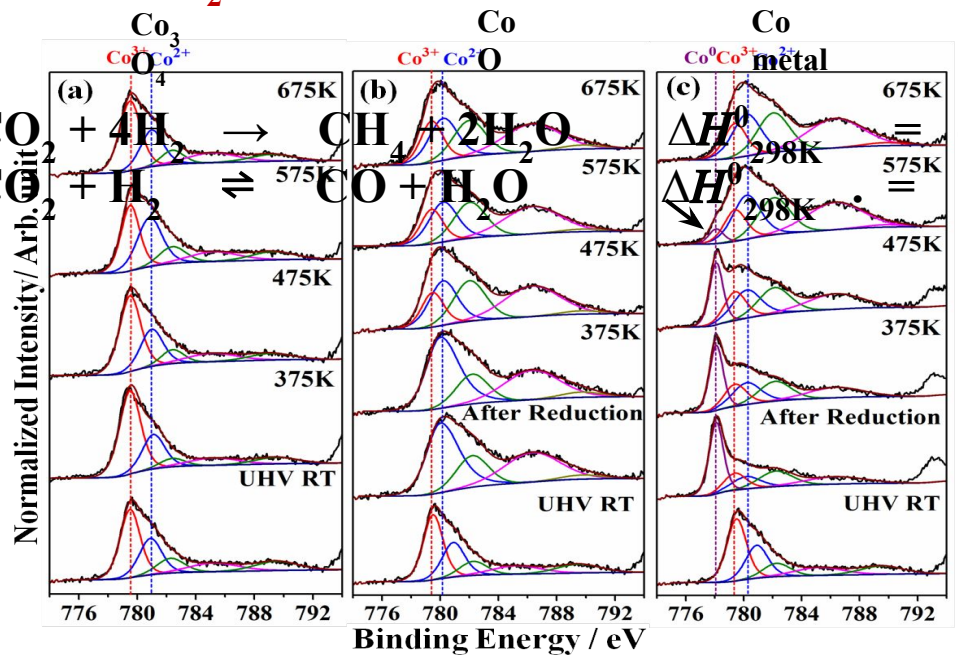
1. **Ravi Ranjan** , Nitin B. Mhamane, Sadhu K. Kolekar, and Chinnakonda S. Gopinath., Electronic Structure Evolution from Metallic Vanadium to Metallic VxOy: A NAPPES Study for O_2 + V Gas–Solid Interaction, J. Phys. Chem. C **2022**, 126, 45, 19136-19146.
2. **Ravi Ranjan**, Jyoti Tekawadia , Ruchi Jain, Nitin B. Mhamane, Thirumalaiswamy Raja and Chinnakonda S. Gopinath, Co_3O_4 for sustainable CO_2 reduction and possible fine-tuning towards selective CO production, Chem. Eng. J., **2023**, 471, 144459.
3. **Ravi Ranjan**, and Chinnakonda S.Gopinath, Nanostructured Ni-Co Core-Shell Catalysts for CO_2 Hydrogenation Explored through NAPPES (Manuscript about to submit).
4. **Patent:** Thirumalaiswamy. Raja, Chinnakonda. S. Gopinath, Nitin .B. Mhamane, and **Ravi Ranjan**, A catalyst for the conversion of CO_2 to CO and process for the preparation thereof, PCT No. WO2023/058057 A1.

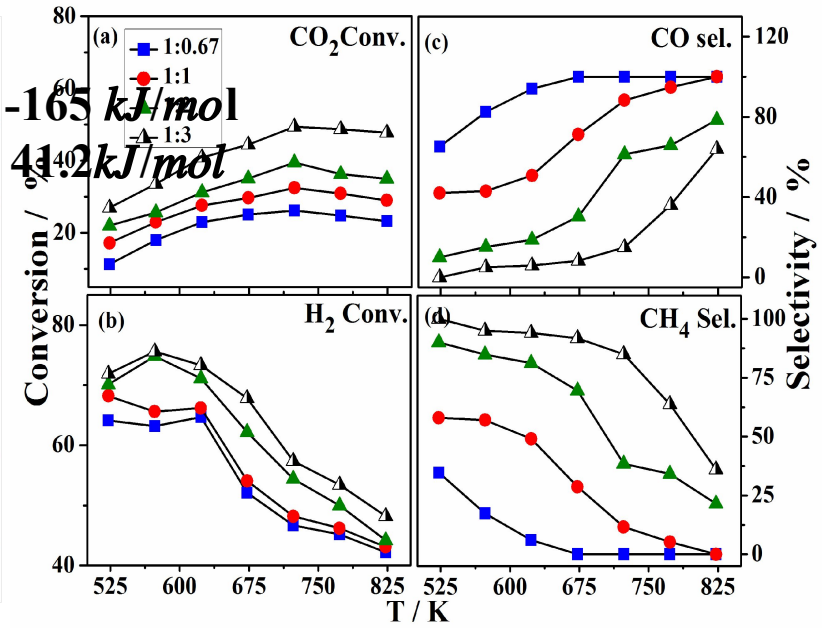
Co_3O_4 for sustainable CO_2 reduction and possible fine-tuning towards selective CO production

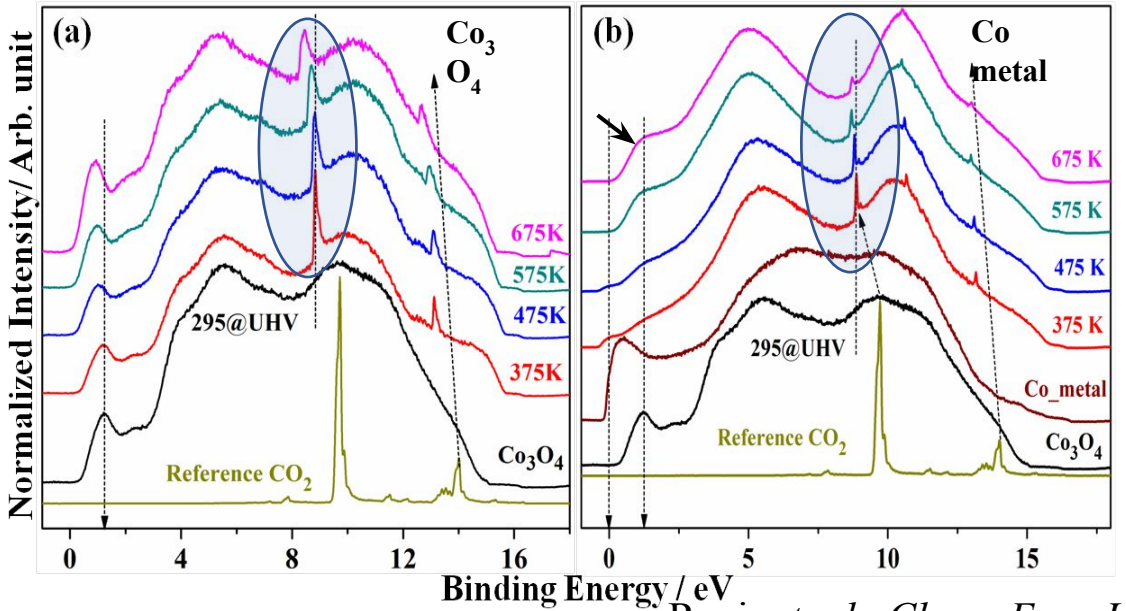


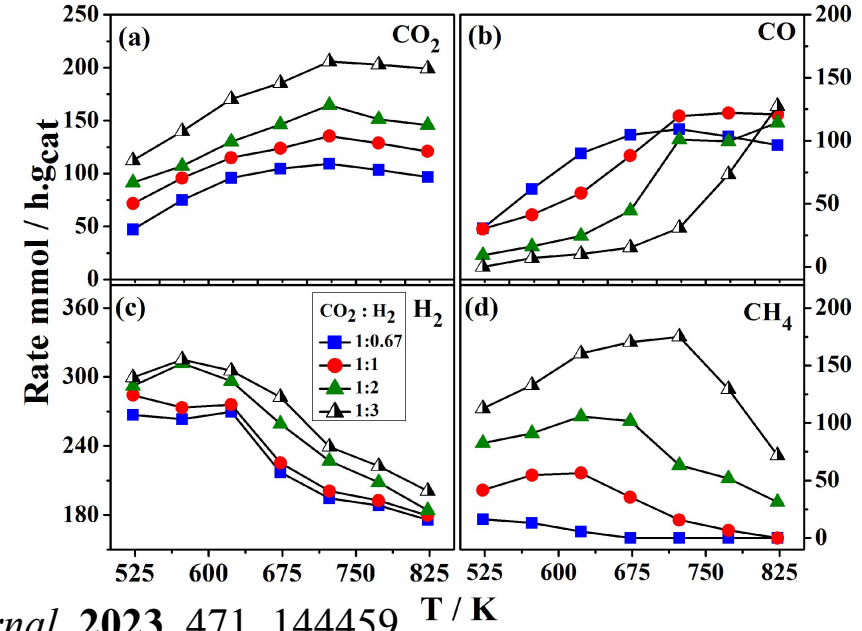
$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O \quad \Delta H^0_{298K} = -165\ kJ/mol$$

$$CO_2 + H_2 \rightleftharpoons CO + H_2O \quad \Delta H^0_{298K} = 41.2\ kJ/mol$$

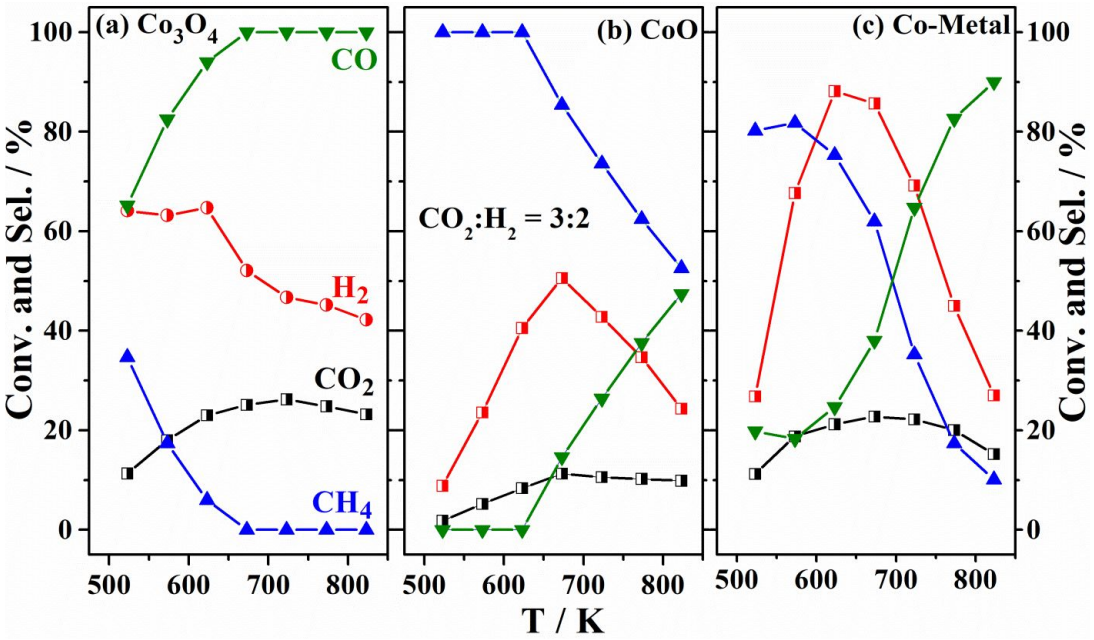


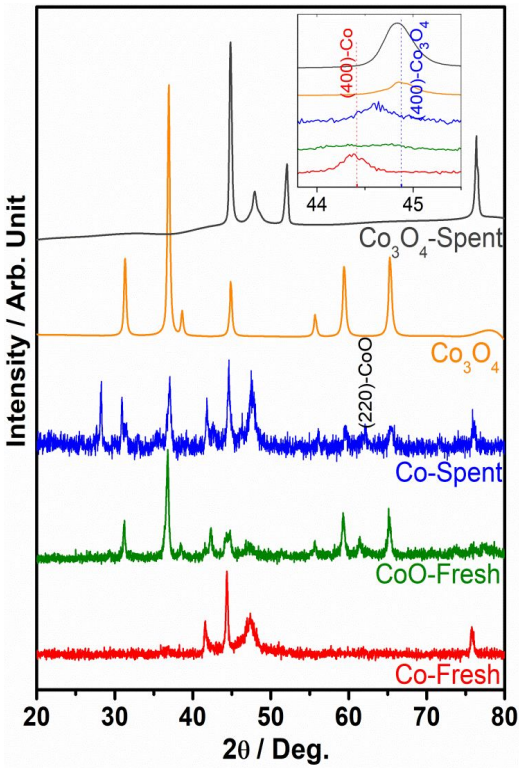


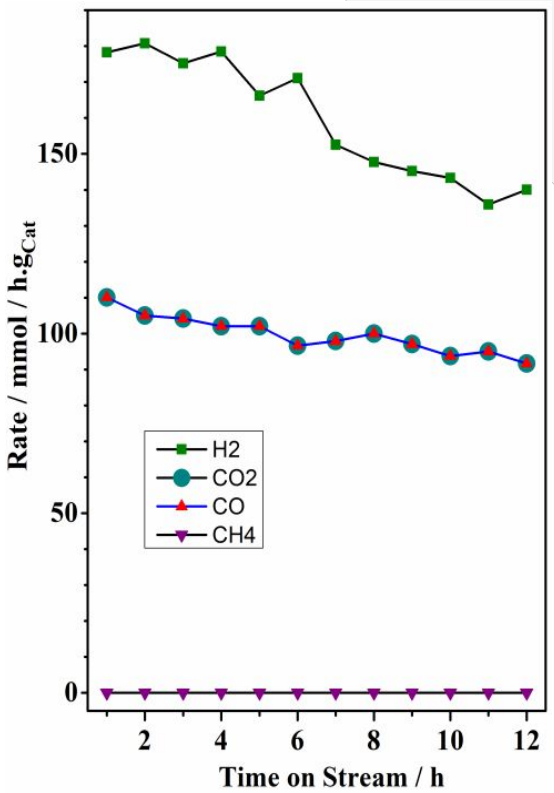




Ravi *et. al.*, *Chem. Eng. Journal*, **2023**, 471, 144459







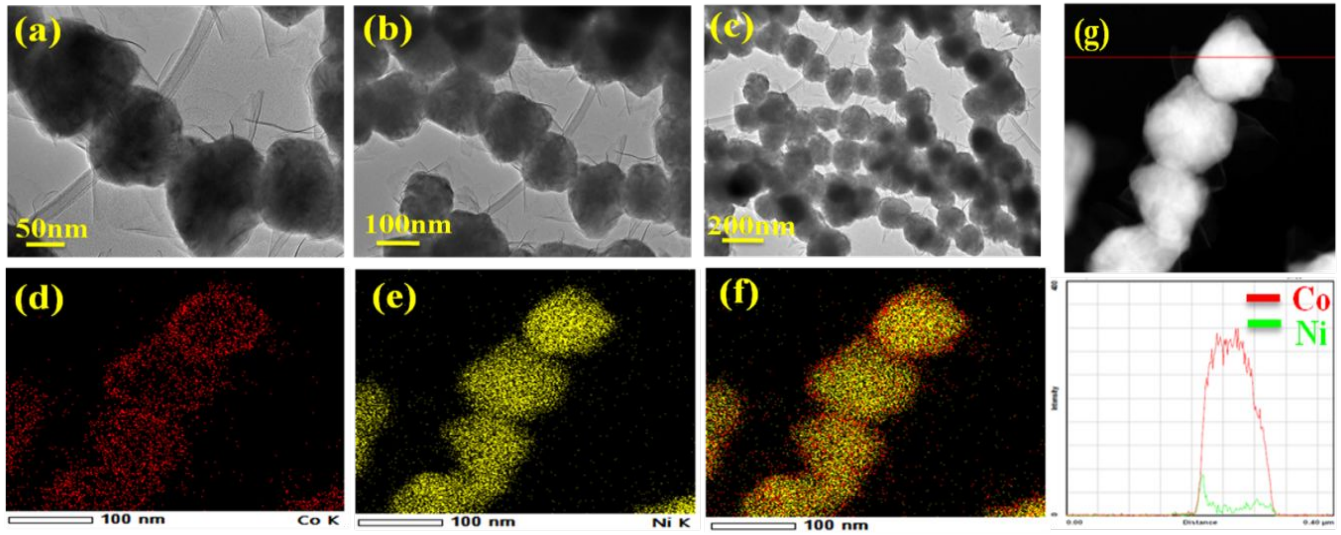
Conclusion

We investigated the surface chemistry and catalysis aspects of Co_3O_4 NC for CO_2 reduction using NAP-XPS, UPS and fixed bed reator.

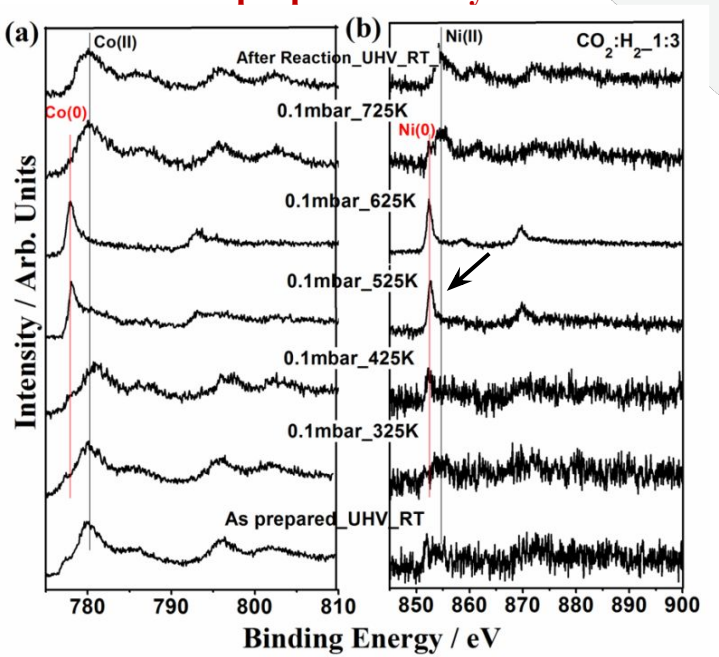
Direct correlarion was observed between the finding of NAPPES at 0.1 mbar partial pressure and catalysis at 1bar along with XRD and TEM characterization.

Ravi *et. al*., *Chem. Eng. Journal*, **2023**, 471, 144459

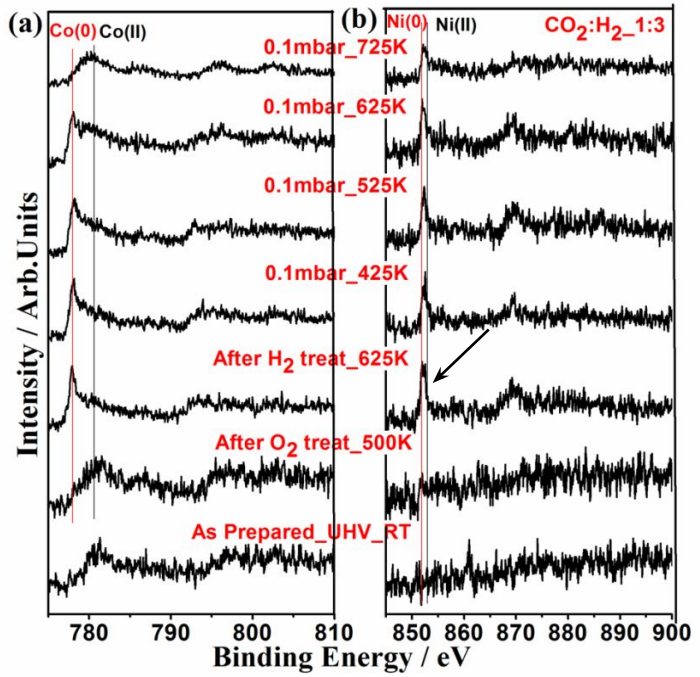
Ni-Co Core-Shell Nanoparticles for CO_2 Reduction reaction: Insights from NAPPES



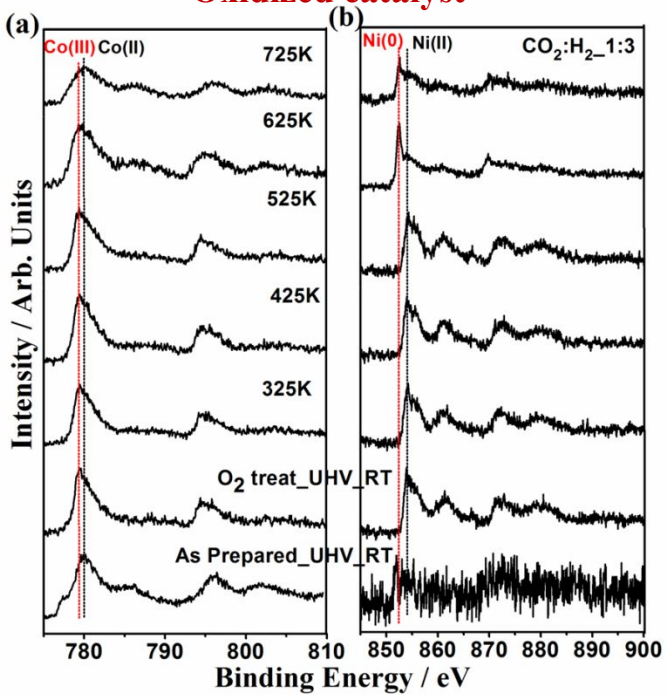
As prepared catalyst

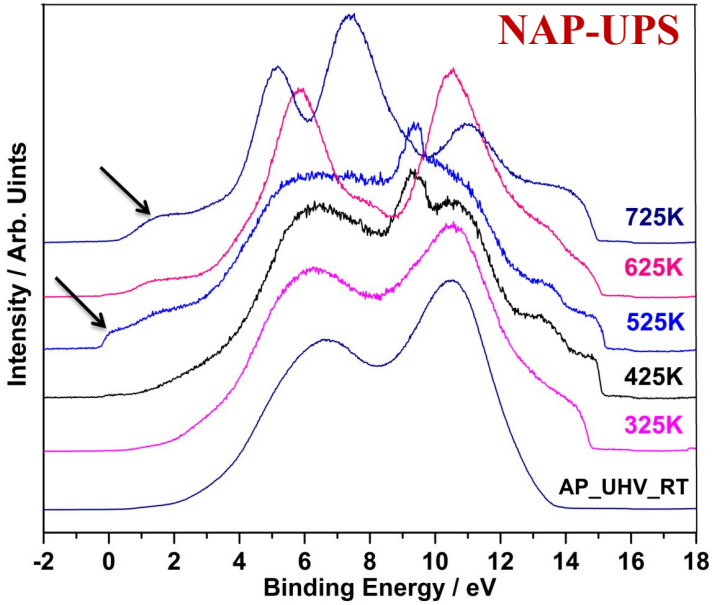


Reductive pretreated catalyst



Oxidized catalyst

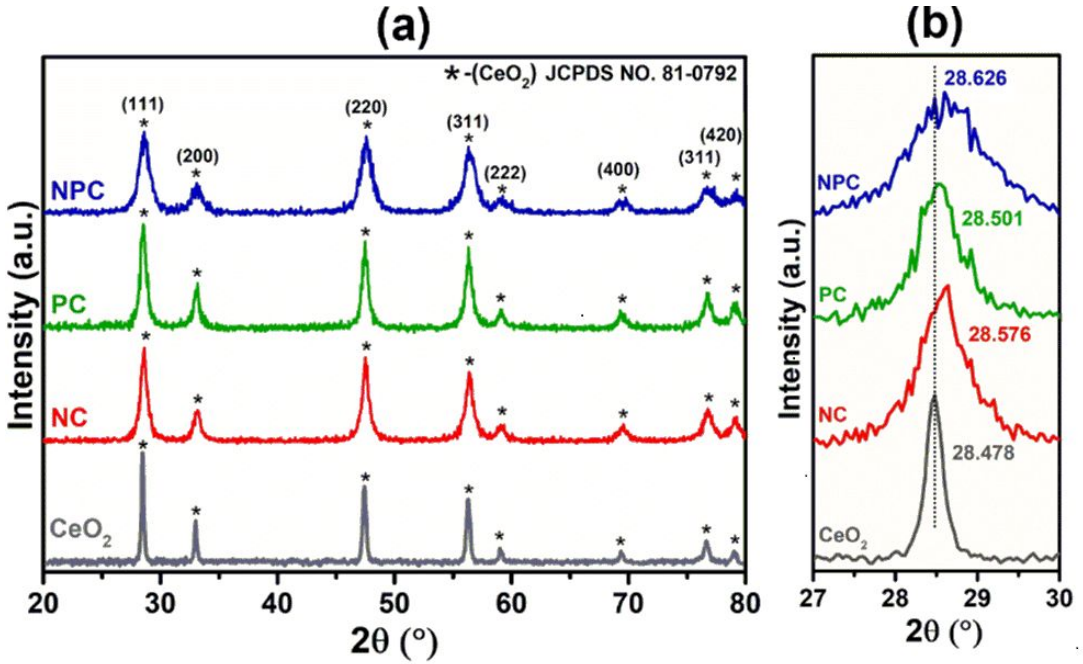


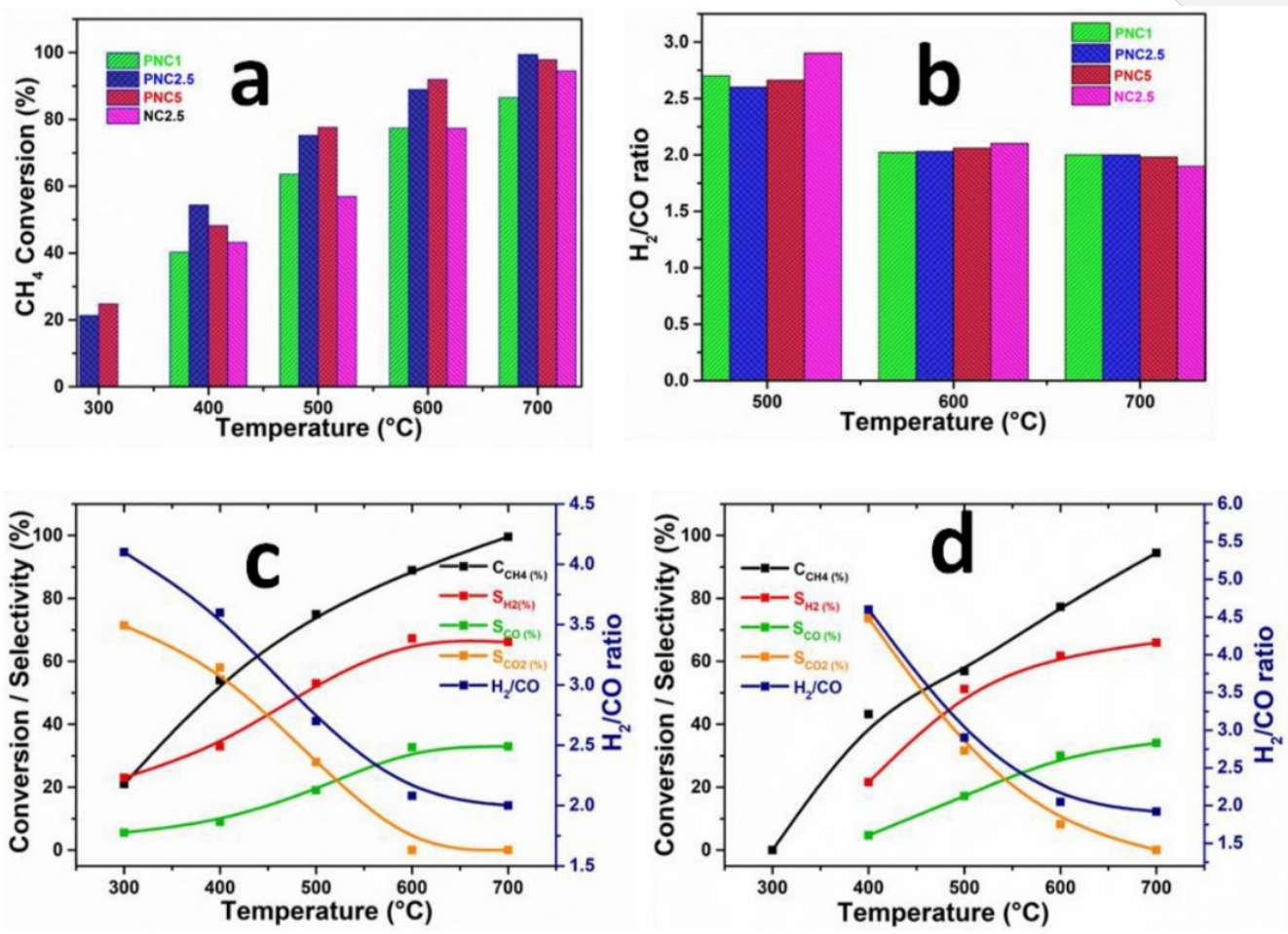


Proposed idea for in-house

Impact of Platinum on Coke Resistance and Stability in Partial Methane Oxidation over Pt-Ni/CeO_2 Catalysts at optimum temperature

2.5 %Ni/CeO_2 (NC2.5), 0.5%Pt/CeO_2 (PC) and 0.5%Pt-2.5%Ni/CeO_2 (PNC2.5)





PNC2.5
Conversion >99%
Stability for 500 h

NC2.5
Conversion ~92%
Activity loss by 66%

R. Khatun *et. al.*, Catal. Sci. Technol., 13 (**2023**), 6431
R. Khatun *et. al.*, Applied Catalysis B: Environmental, 340 (**2024**) 123243

Expected outcomes

- To understand the active mechanism of CH_4 partial oxidation and provide evidence for the superior redox behavior of Ni-Pt bimetallic catalysts compared to monometallic Ni and Pt catalysts
- The synergy between Pt and Ni and understanding the critical role of oxygen vacancy sites (V_o) in the ceria lattice in enhancing catalytic activity at low temperatures
- The study will identify the specific Ni and Pt species that serve as active sites for CH_4 activation and O_2 dissociation, analyzing their redox changes under reaction conditions
- It will also confirm the critical role of the CeO_2 support, particularly the Ce^{4+}/Ce^{3+} redox pair's involvement and its role in stabilizing Ni and Pt cationic states at the interface
- The research will examine the changes in the electronic structure of both the surface and bulk of the catalysts through combined XPS/XAS analysis under realistic conditions (up to 5 mbar)

Goals for the ALBA Stay:

- **Proven Skills:** Expertise in catalyst development for gas phase reactions, strong research publication record with 11 papers during Ph.D., and significant contributions to the field of heterogeneous catalysis and surface science

- **Motivation:** Tackling climate change through nanomaterials that improve efficiency and effectiveness in carbon conversion technology

- **Key collaborators and Networking:**

✔ Built scientific connections with key scientist in the related filed.

✔ Established connections with researchers and professionals at ALBA and outside ALBA, fostering collaborations and sharing knowledge in the scientific community.

1. Dr. Samuli Urpelainen, University of Oulu, Finland
2. Dr. Manoj Kumar Ghosalya, University of Oulu, Finland
3. Dr. Rajaram Bal, Senior Principle Scientist and Professor (AcSIR) at CSIR-IIP, India
4. Dr. Kanak Roy, Assistant Professor at Banaras Hindu University, Varanasi, India
5. Dr. (Prof) Chinnakonda S. Gopinath, Visiting Professor at IIT, Palakkad, india

- ✔ Within CIRCE-NAPP, planning to apply for funding to "**Plan Nacional" calls**, in collaboration with selected user groups, to raise funds for key experimental developments and inhouse research funding
- ✔ Planning to attend **and organize** workshops and seminars to expand connections in the scientific national and international community

❑ Approach:

- ✔ Utilize state-at-the-art facilities at ALBA for materials characterization and operando studies
- ✔ Implement the experimental approach to understand catalyst behavior
- ✔ Building communication with collaborators to exchange ideas and experimental design

❑ Long term Goal:

- ✔ Gaining a deeper understanding of the mechanistic aspects of catalysts in solid-gas reactions, along with mastering new techniques, data interpretation and also explore the soild-liquid interactions
- ✔ Aiming to publish novel findings in reputable journals and present at conferences
- ✔ Additionally, contributing to the advancement of CIRCE-NAPP instruments by implementing updated methods and technology, enabling users to push the boundaries of NAPP instrumentation

Summary

- Previously focused on real-world catalysts, my aim to further explore innovative catalysts to advance the field of catalysis for societal benefit
- Planning to strengthen the catalysis capabilities at ALBA, build collaborations and networks with users, and encourage research groups to utilize synchrotron facilities for their experiments
- Generate ideas for in-house initiatives and the ALBA open house, and collaboratively develop a research proposal for the open house in partnership with collaborators
- Additionally, I intend to deepen my expertise in data interpretation and broaden my knowledge of emerging instrumental techniques


Thank You