catCHy

EUROPEAN TRAINING NETWORK

Novel catalysts for $CO_2$ Hydrogenation and Electro-reduction

MŰEGYETEM 1782

## Mid-term review meeting

# DFT-based theoretical modelling of the catalytic activity of deposited clusters.

Bárbara Zamora Yusti

Supervised by Prof. László Nyulászi and Prof. Tibor Höltzl

ESR6

Budapest, April 22nd of 2022

# Experience

Master of Science, MSc (Synthesis, Catalysis and Molecular Design), URV.

Chemist with experience in:

- Computational Photochemistry

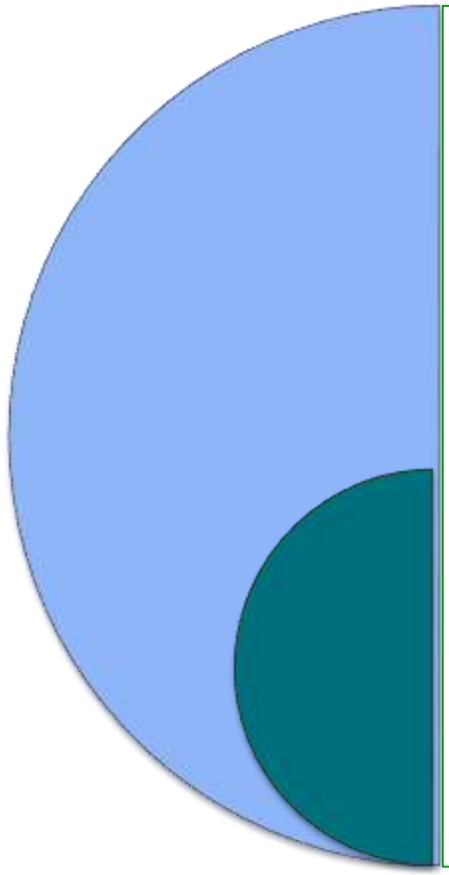
- Atomic and molecular structure

UNIVERSITAT ROVIRA i VIRGILI

Quantum Chemistry Group

Universidad del Valle

# Objectives (as part of WP3 and WP4)



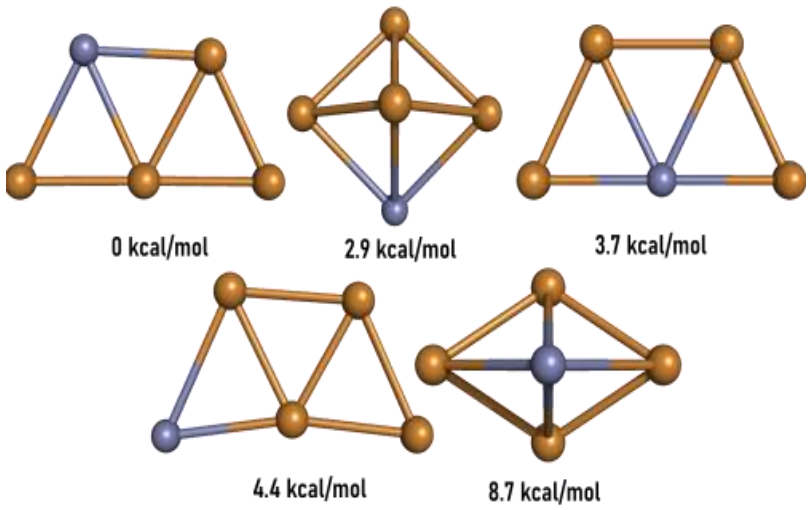
**Methodology**

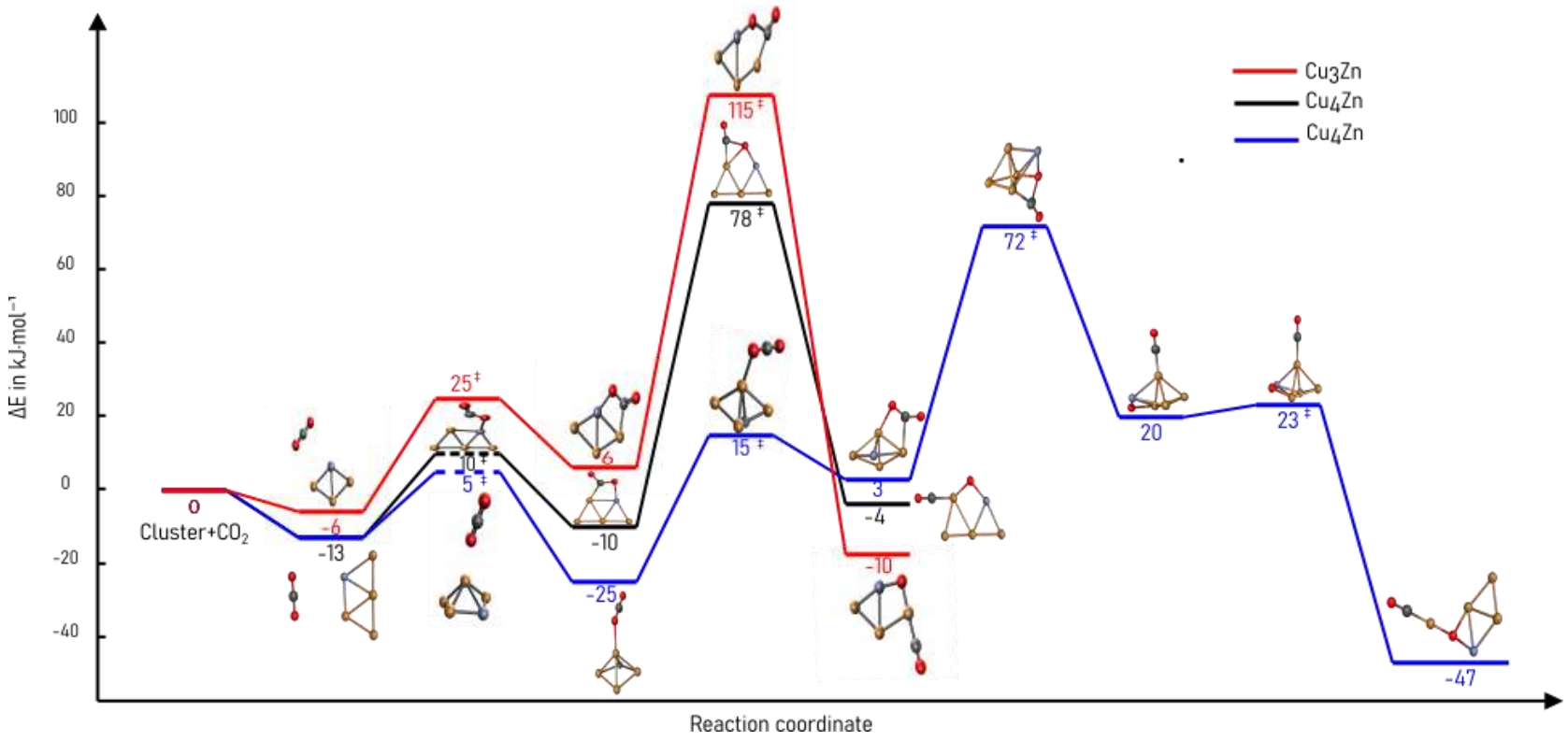
To select the method of the calculations, test, benchmark and compare to available experiments on small CuZn clusters.

**System of study**

To provide an adequate description of the mechanism of $CO_2$ activation on CuZn clusters. Perform calculations expanding the number of copper atoms from n=4 to n=6.

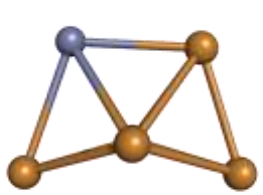
# Results $Cu_4Zn$



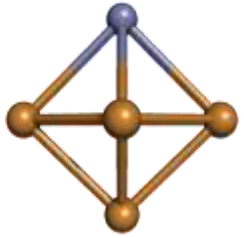




Szalay, M. et al. *Phys. Chem. Chem. Phys.,* **2021**, 23(38), 21738-21747

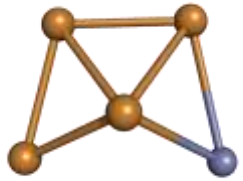
# Results $Cu_5Zn$



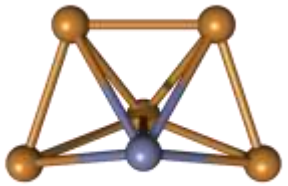
0 kcal/mol



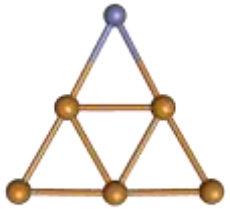
0.4 kcal/mol



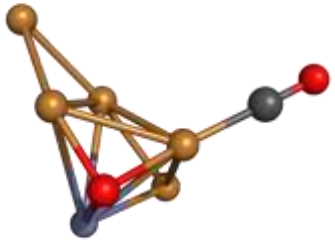
1.6 kcal/mol



2.3 kcal/mol

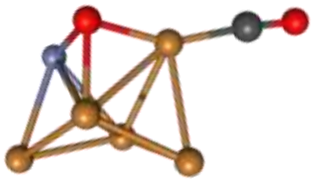


16.3 kcal/mol

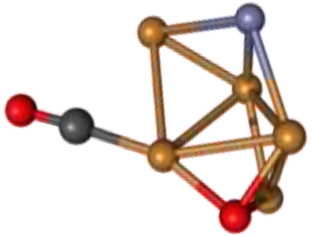


0 kcal/mol

1.4 kcal/mol



5.2 kcal/mol



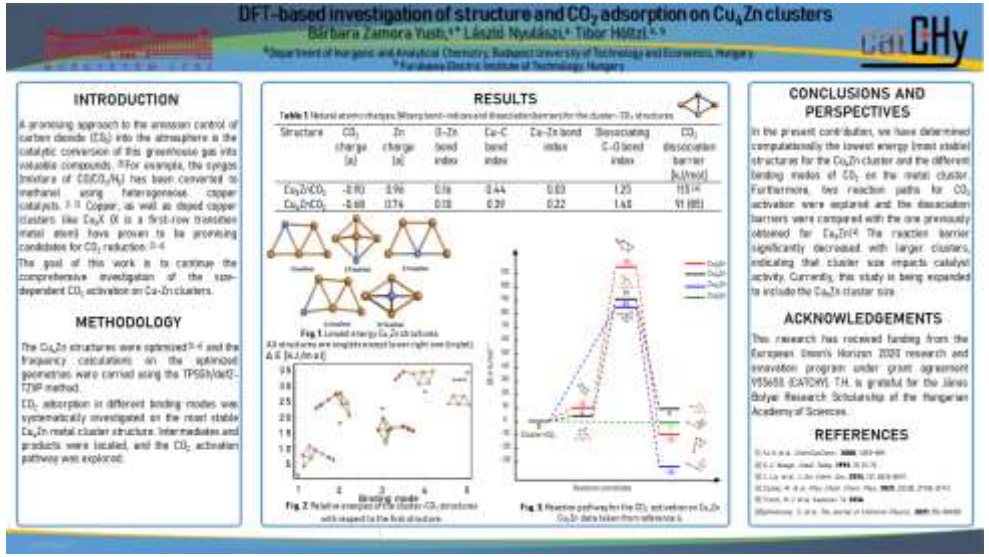
8.5 kcal/mol

# Training

| Objective | Action |
|---|---|
| Research skills | Courses: modern computational chemistry and inorganic chemistry.<br>Seminars organized by the George Oláh doctoral school: open science practices and publishing scientific results. |
| Language, writing and communication | Hungarian course and poster presentation. |
| Teaching | General chemistry laboratory and general chemistry calculations. |

# Outreaching

Poster presentation in the workshop **Cutting-Edge Homogeneous Catalysis** (CEHC-2) (29-31 March 2022) and at the **First Catchy School** (19-21 April 2022)



# Secondments

| Project title | Date |
|---|---|
| RU for training on IR vibrational spectroscopy of cluster-molecule complexes. | October-November 2022 |
| KUL for TPD measurements to study deposited cluster reactivity. | March-April 2023 |
| VITO for modelling of catalysts under realistic reaction conditions. | March-April 2024 |

# Thank you for your attention