- Born in Italy in 1996
- 2015-2021 Physics studies (BSc, MSc) in Germany, at the Free University Berlin
- Specialized in molecular Physics and Markov Modeling

My works:

- Sechi, R. et al, Multiscale Modeling & Simulation 2021 19:2, 758-774
- Sechi, R. et al, Proc. Appl. Math. Mech., 2021, 21: e202100102
- Sechi, R.et al, SepFree NMF: A toolbox for analyzing the kinetics of time-resolved spectra, *submitted*

Secondments:

- University of Ulm in 2022
- PSI in 2023

In CatCHy:

- Work at FETI and studying&teaching at BME
- Member of WP3 and WP4

In CatCHy:

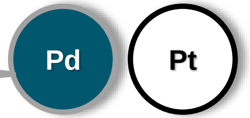
- Simulation of CO_2 electroreduction with DFT and other quantum chemistry methods

Systematic study:

Small clusters in vacuum -> add CO2 -> add solvent -> add surface -> study bigger clusters -> add potential

Compare to experiments at each step

The clusters I am studying



catCHy

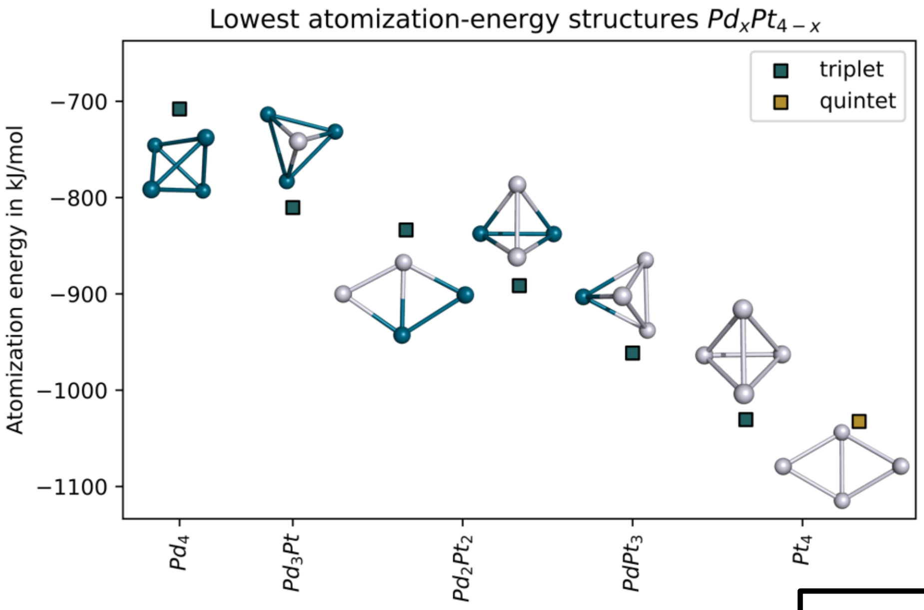
EUROPEAN TRAINING NETWORK

Novel catalysts for CO2 Hydrogenation and Electro-reduction

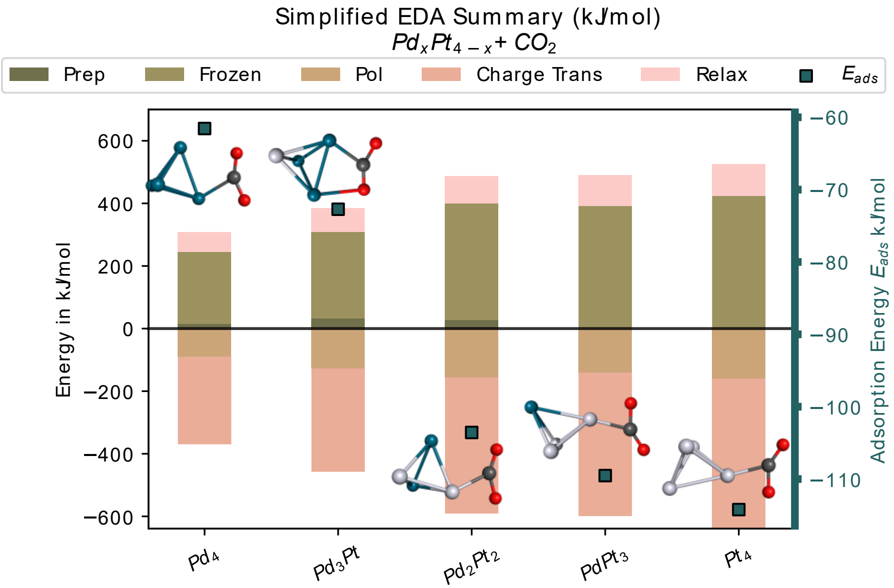
FURUKAWA ELECTRIC INSTITUTE OF TECHNOLOGY

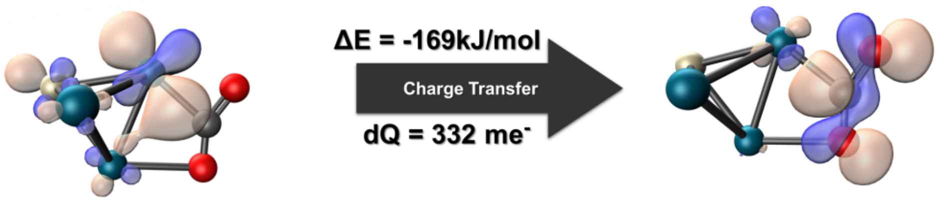
DFT study of CO_2 adsorption of $Pd_xPt_{(4-x)}$ clusters in the gas phase

Most stable structures



Energy decomposition Analysis





- Palladium doping of platinum clusters tunes the CO_2 reactivity of the cluster
- The d-orbital of the transition metal transfer charge to the π* system (LUMO) of the CO_2

Pd Pt

Renata Sechi, ESR5 Catchy School Budapest 19-22 April 2022

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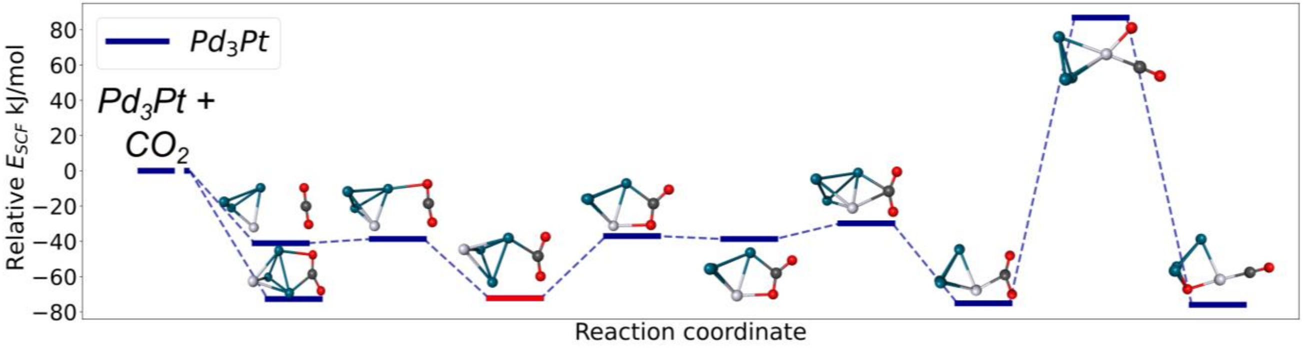
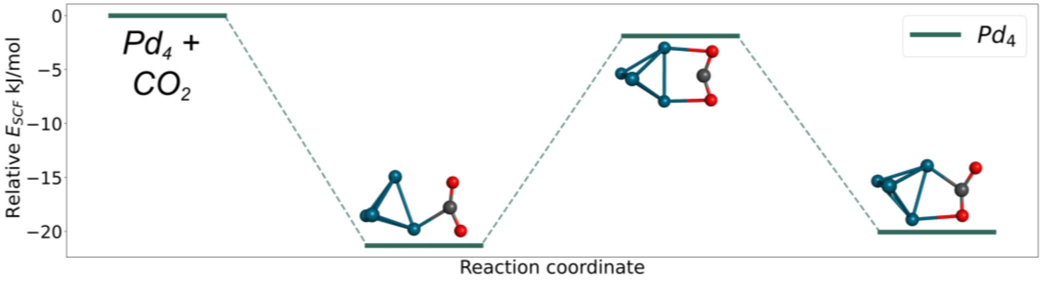
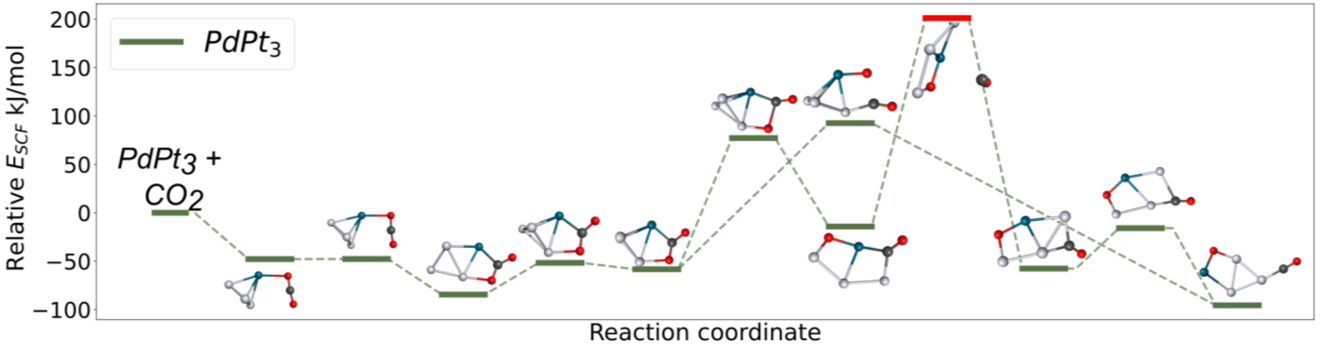
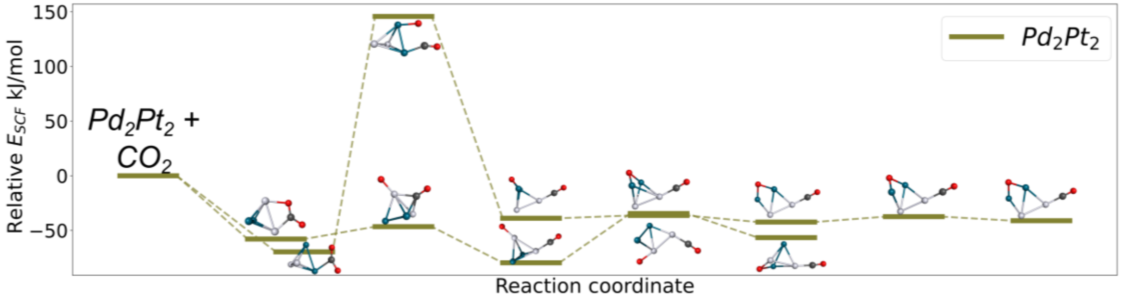
Novel catalysts for CO_2 Hydrogenation and Electro-reduction

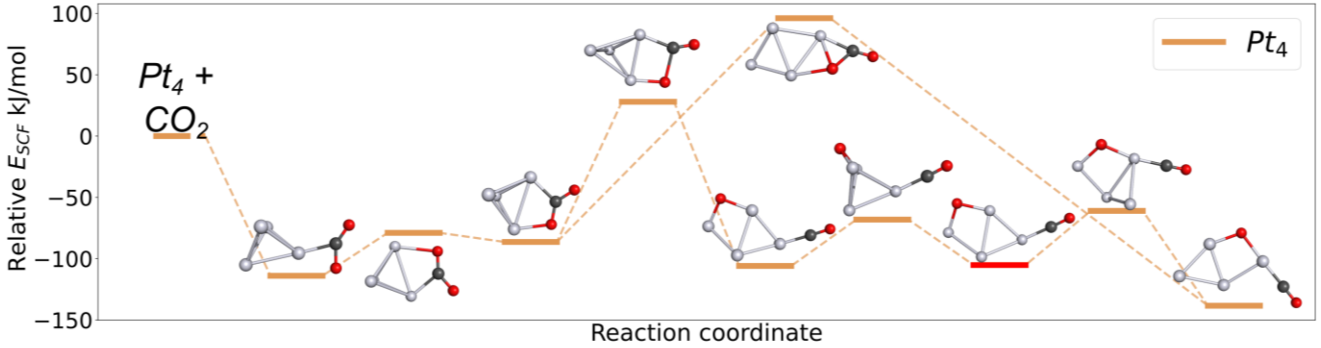
FURUKAWA ELECTRIC INSTITUTE OF TECHNOLOGY









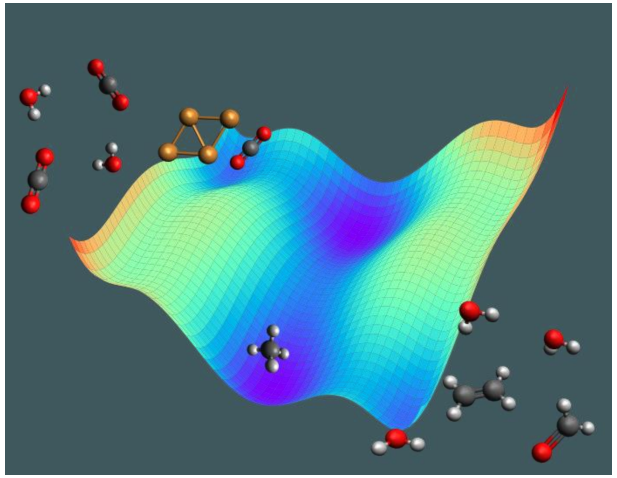


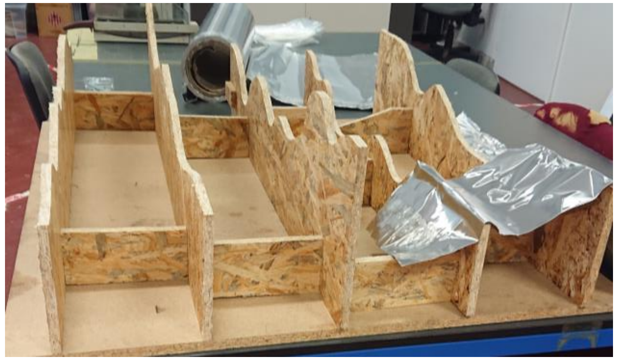
Outreach:

- European Researchers Night 2021: Blowing CO2 away, built at FETI

Conferences (online)

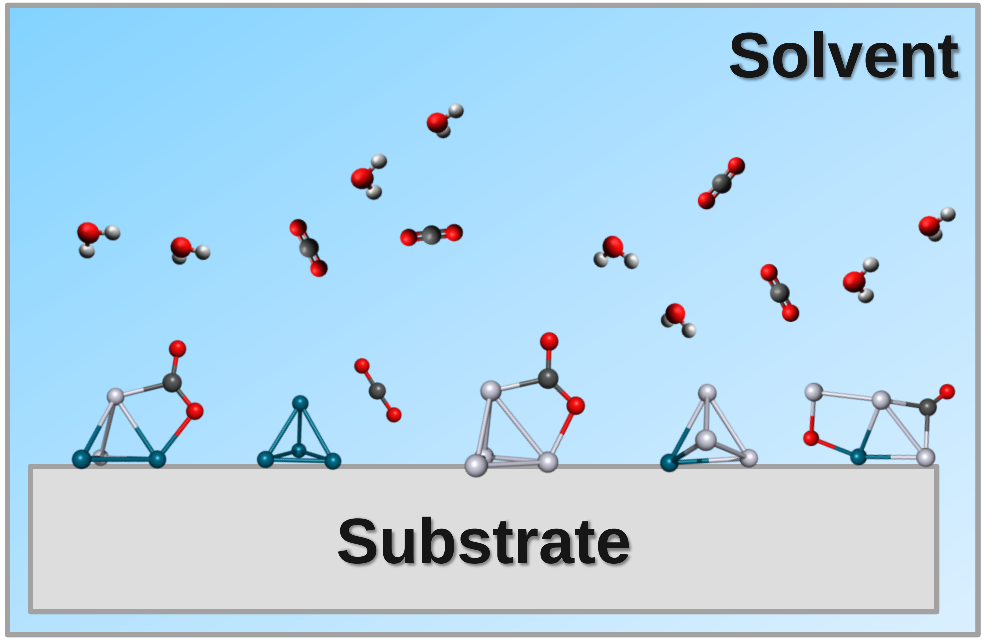
- Presentation of a poster at CEHC 2022 in Leipzig, Germany





Future Plans

- Further investigation of $Pd_xPt_{(4-x)}$ reaction paths
- $Pd_xPt_{(4-x)}$ clusters on substrate + solvent
- Simulation of bigger cluster
- Integration of information + comparison with experimental results (University of Ulm, University of Antwerp, PSI)



Partecipation to CatCHy Schools and Conferences

Pd Pt