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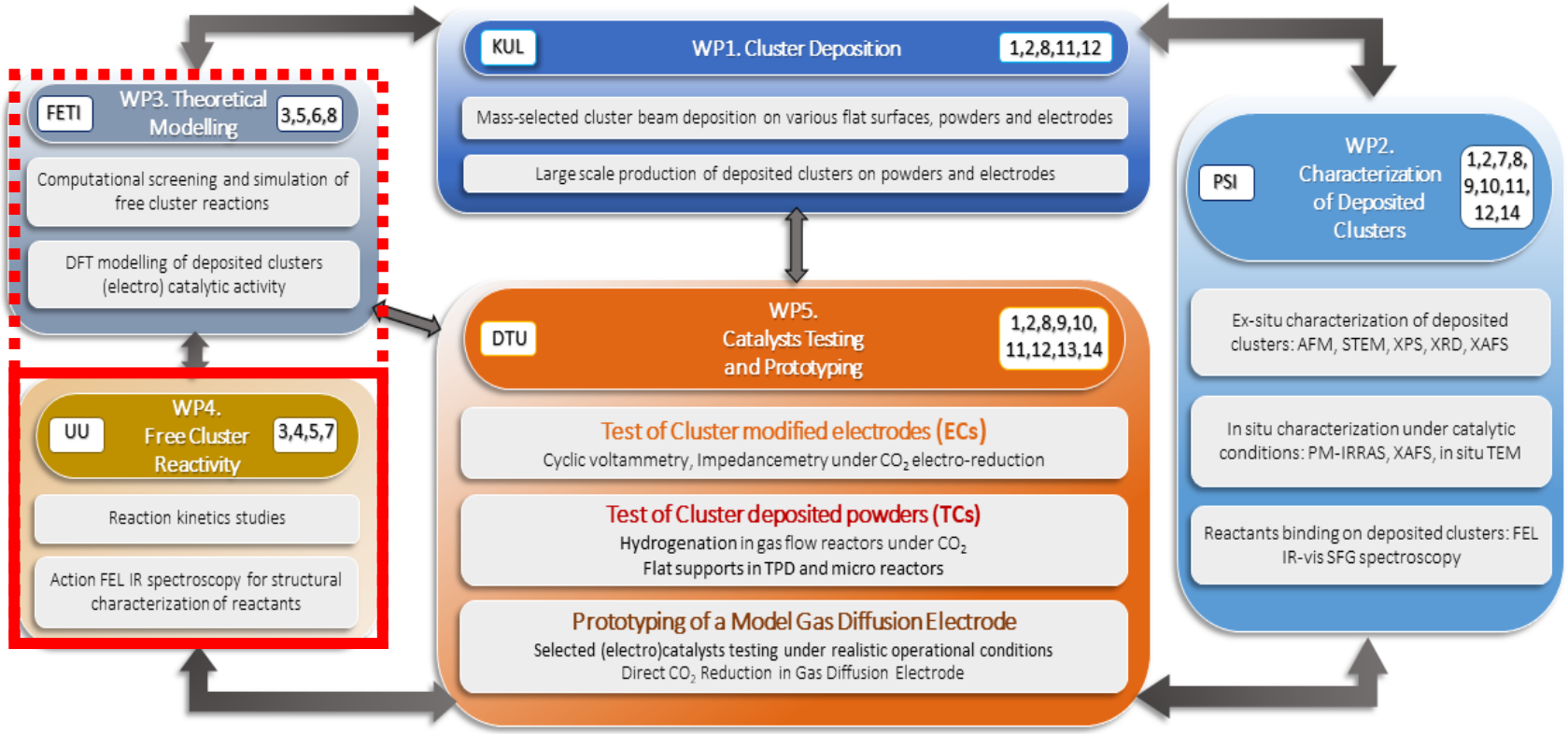


Aim: Study of Interaction between free [mono-/bi-]metal oxide clusters and CO_2 , H_2 based on

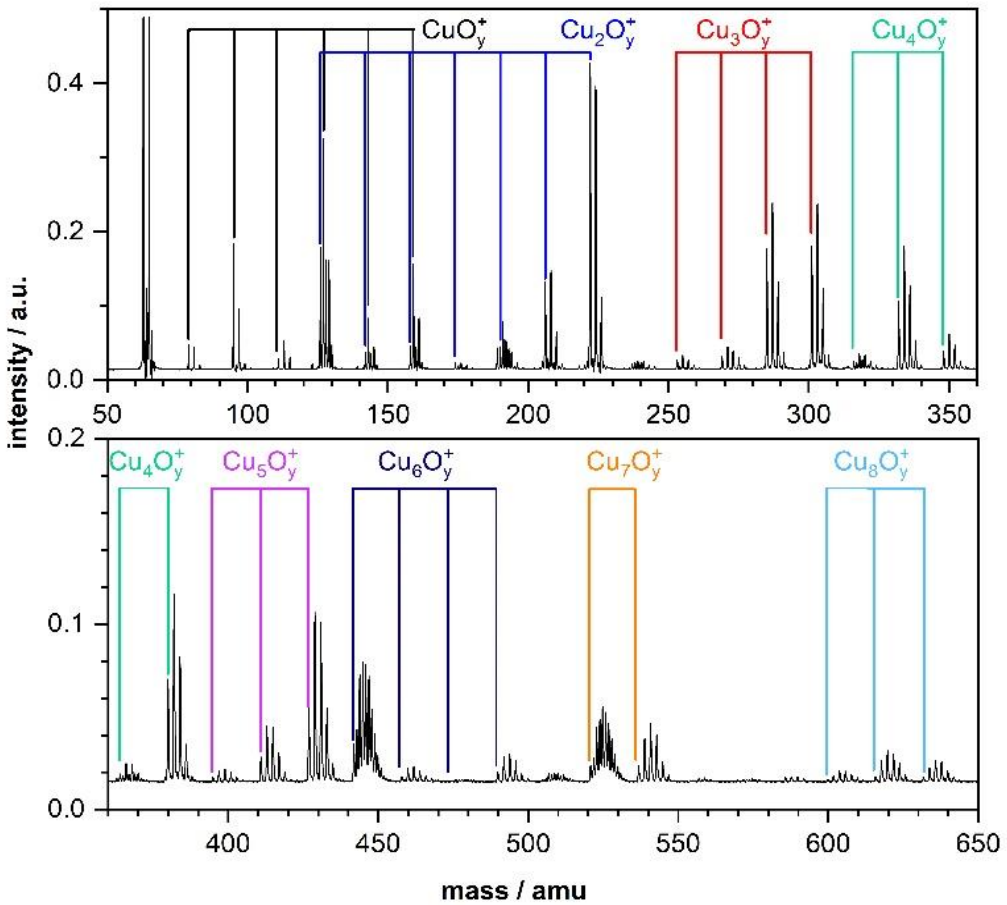
- Cluster size
- oxygen content

FURUKAWA ELECTRIC GROUP

Cluster mass spectra

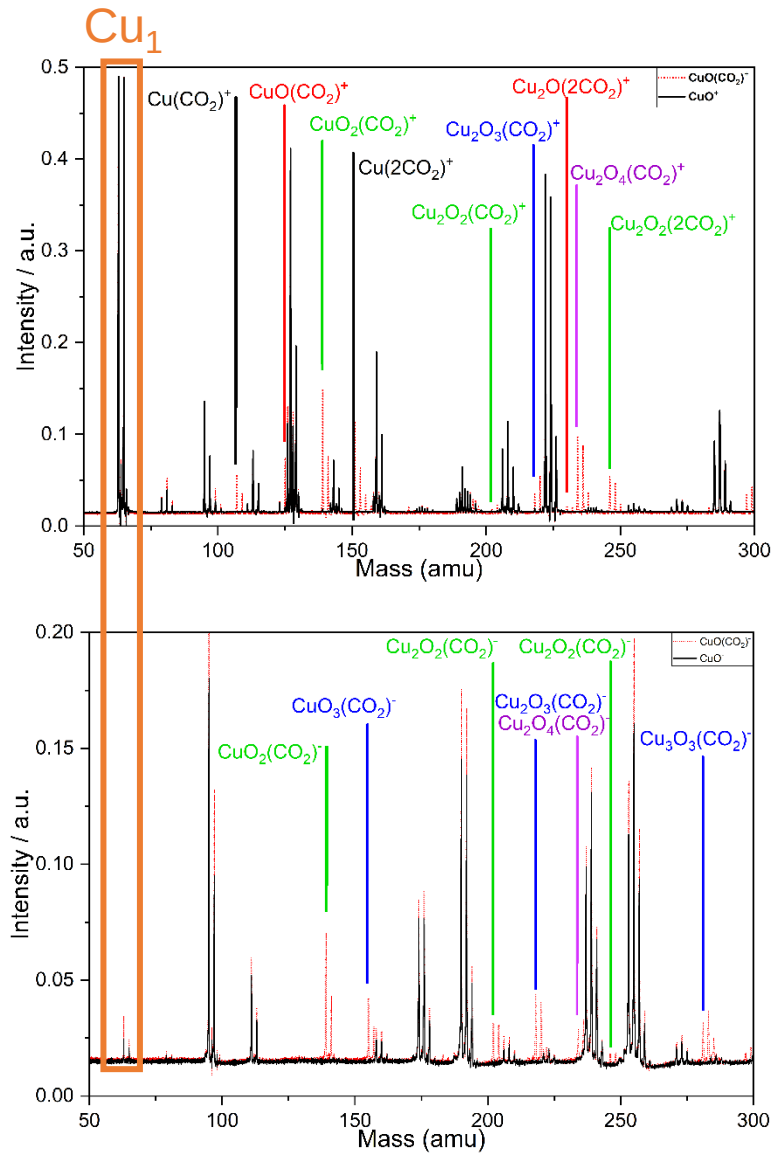
Mass spectrum of copper oxide clusters

D4.1	1st report on mass spectra of metal-oxide clusters with different metal/ oxygen ratios	WP4	UU	R	CO	M12



Mass spectrum of CATIONIC copper oxide and CO_2 clusters

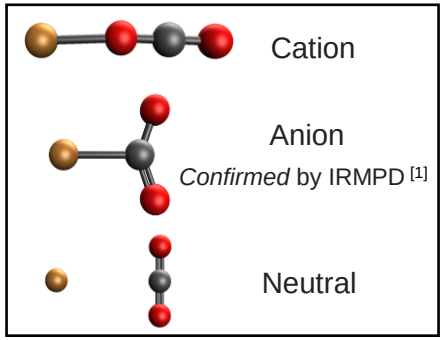
Mass spectrum of ANIONIC copper oxide and CO_2 clusters



Optimized geometries of Copper oxide species

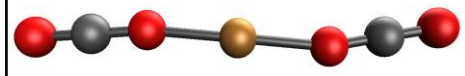
Single Cu atom much more abundant in cation form*

+ CO_2



= Copper
= Oxygen
= Carbon

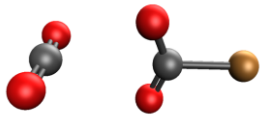
+ 2 CO_2



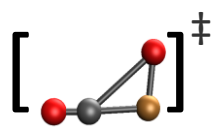
Cation - Present in the spectra

CuO_4C_2 (Cu ; 2CO2)

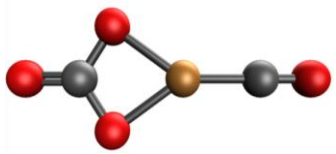
Anion – Not present



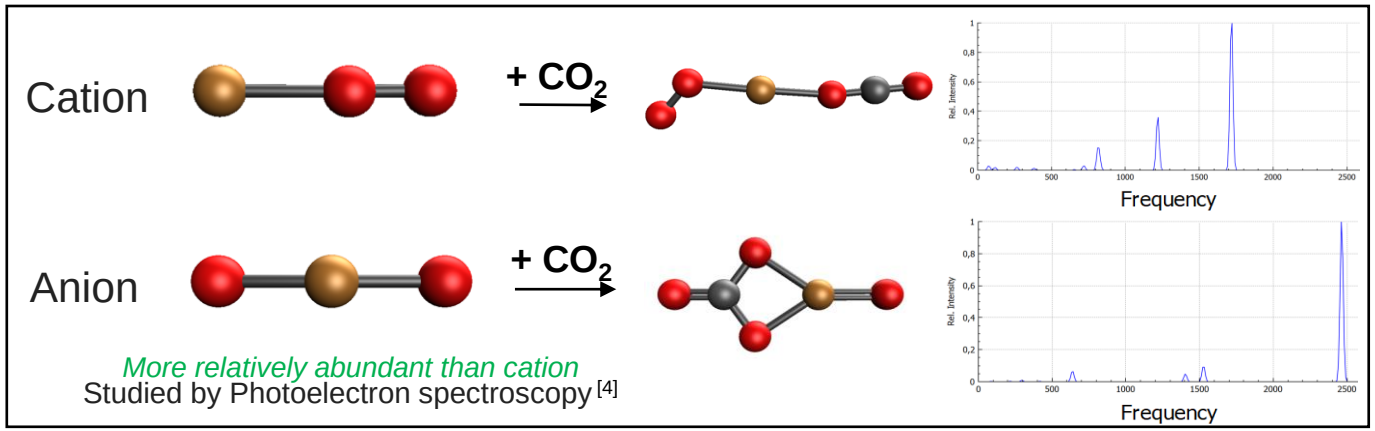
Confirmed by IRMPD [1]



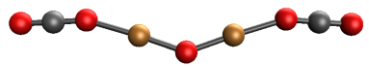
~ 2eV barrier



Lowest energy geometry

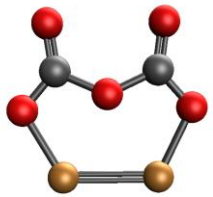


More relatively abundant than cation
Studied by Photoelectron spectroscopy [4]

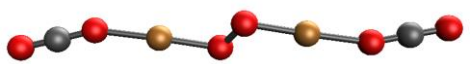


Cation - Present in the spectrum

$Cu_2O_5C_2$ (Cu_2O ; 2 CO2)

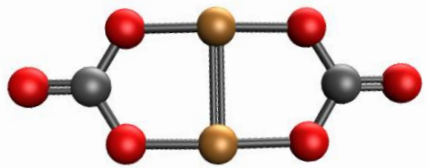


Anion – Not present



Cation

$Cu_2O_6C_2$ (Cu_2O_2 ; $2CO_2$)



Anion

*note that the spectra were obtained by adding oxygen to the system

Structures shown are calculated with:

a) B3LYP hybrid functional with *def2-TZVP* basis set

b) aug-cc-pVTZ for the O atoms, and the *aug-cc-pVTZ-PP* for the Cu atoms [2][3]

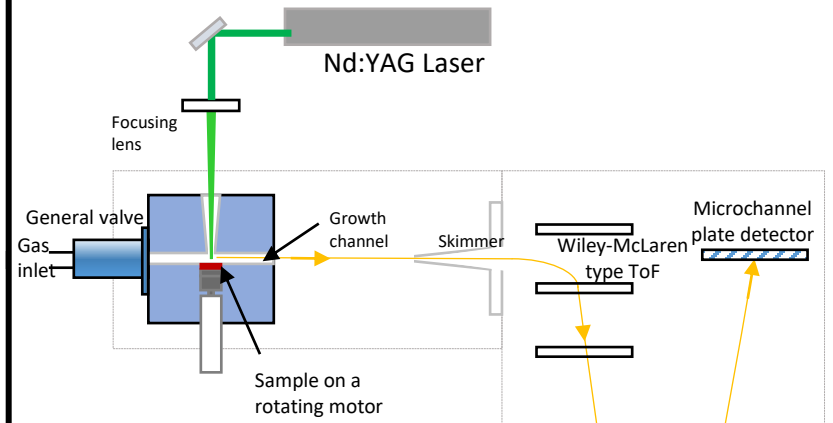
[1] Knurr, et.al., The Journal of Physical Chemistry A **118.44** (2014): 10246-10251.
[2] Yan, Shuai-Ting, et al., The Journal of Chemical Physics **156** (2022): 054304.
[3] Xu, Xi-Ling, et al., Physical Chemistry Chemical Physics **20.31** (2018): 20622-20628.
[4] Chertihin, et. Al., The Journal of Physical Chemistry A **101.22** (1997): 4026-4034.

Going forward

- Calculation of anion and neutral forms of these clusters, and transition states
- Training in investigation of spin densities and bond orders and large clusters
- Working on a laser vaporization Time-of-flight setup and an ion trap setup at Ulm university
- Write a proposal for beam time at FELIX laboratory
- Planned secondment at Radboud University

Radboud University

Laser vaporization cluster source with reflectron time-of-flight detector



Experimental setup with octopole ion trap