5th International Meeting on Materials Science for Energy Related Applications

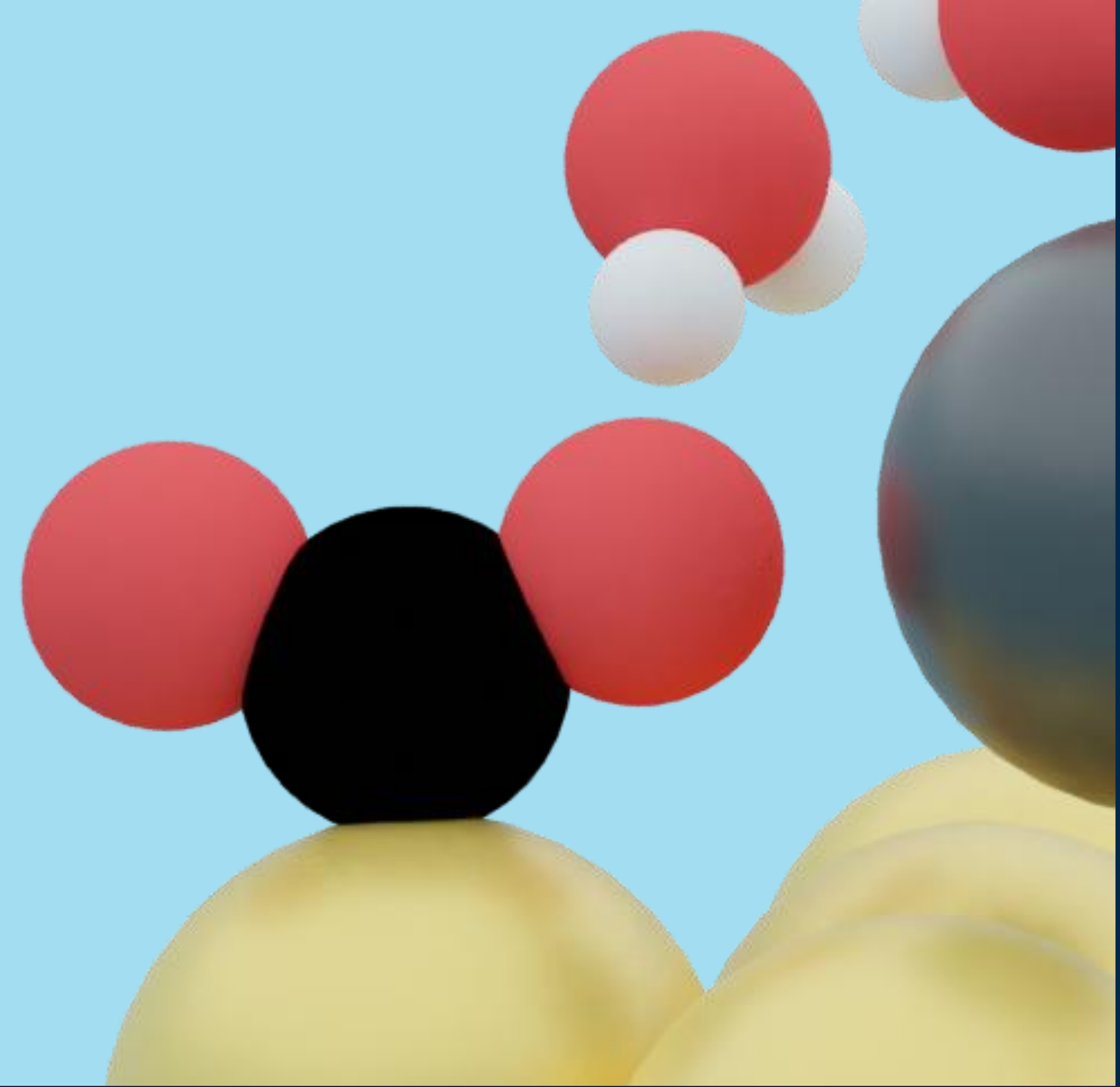
September 25-26, 2025, Belgrade

Automatizing data storage, analysis, and sharing for the electrochemical CO_2 reduction – the FAIR case of SuPERCO2

Dr. Federico Dattila
Department of Applied Science and Technology
Polytechnic of Turin

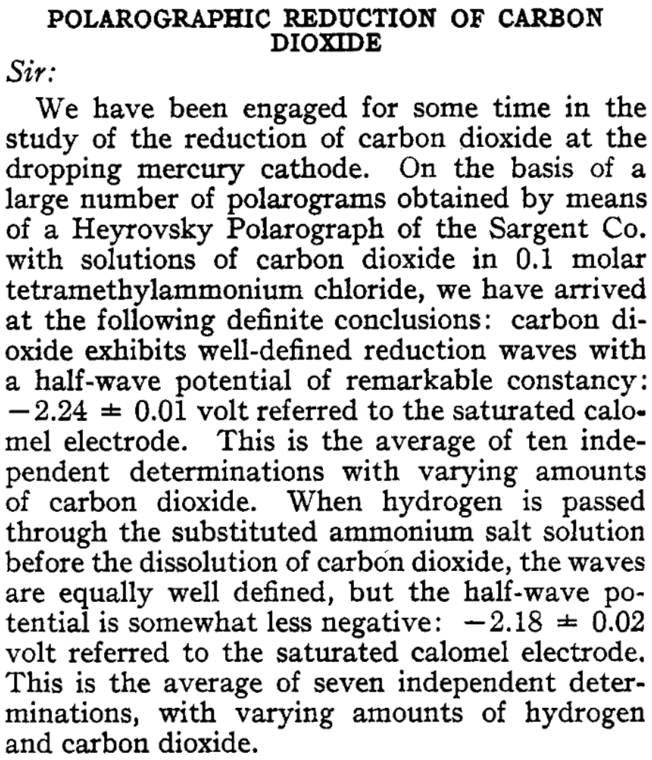
Politecnico di Torino
1859

General meeting – Prof. Simelys Hernández's group
17/10/25, Turin



The FAIR problem of CO_2R

Publications on CO_2R

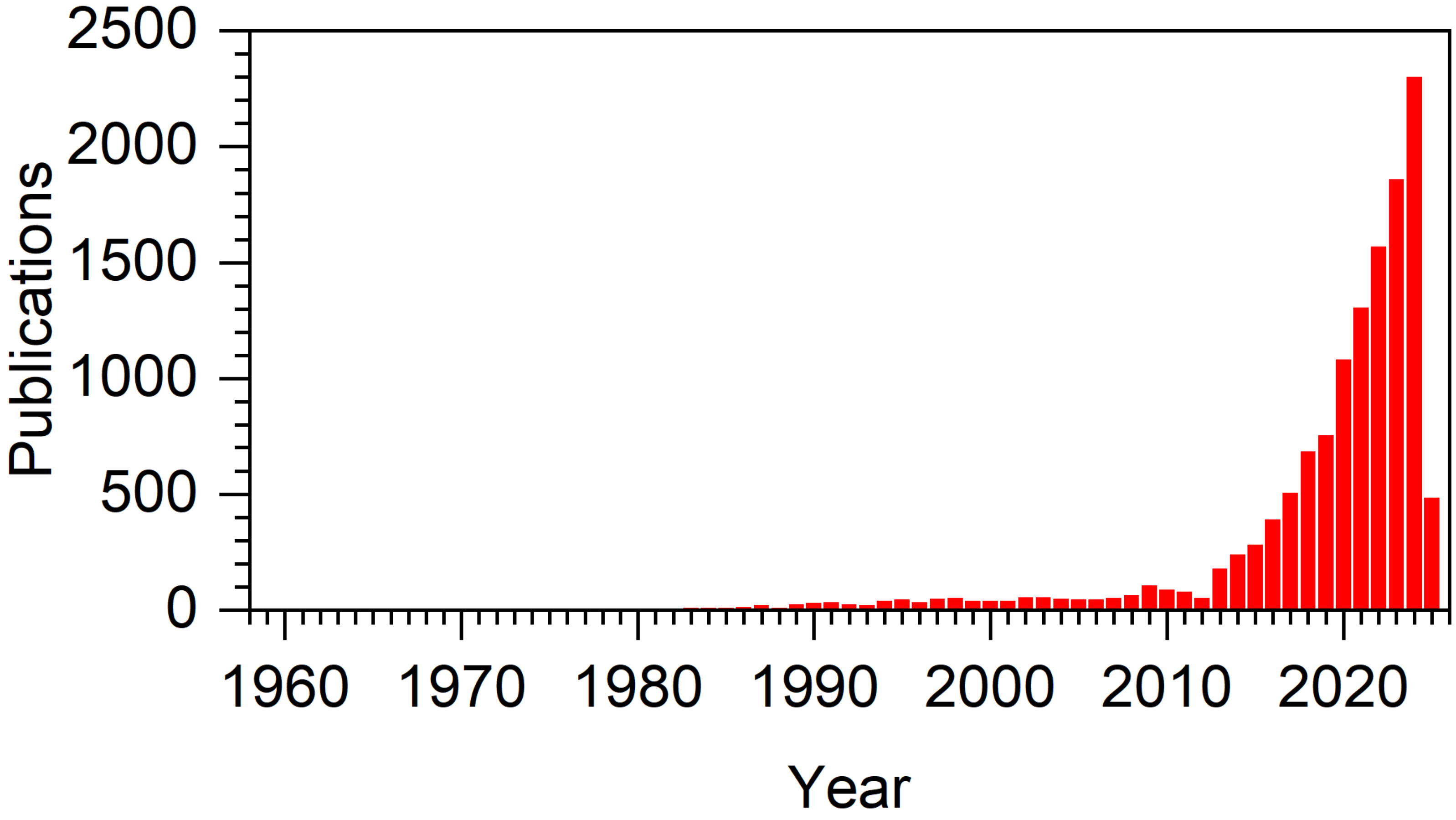


POLAROGRAPHIC REDUCTION OF CARBON DIOXIDE

Sir:

We have been engaged for some time in the study of the reduction of carbon dioxide at the dropping mercury cathode. On the basis of a large number of polarograms obtained by means of a Heyrovsky Polarograph of the Sargent Co. with solutions of carbon dioxide in 0.1 molar tetramethylammonium chloride, we have arrived at the following definite conclusions: carbon dioxide exhibits well-defined reduction waves with a half-wave potential of remarkable constancy: -2.24 ± 0.01 volt referred to the saturated calomel electrode. This is the average of ten independent determinations with varying amounts of carbon dioxide. When hydrogen is passed through the substituted ammonium salt solution before the dissolution of carbon dioxide, the waves are equally well defined, but the half-wave potential is somewhat less negative: -2.18 ± 0.02 volt referred to the saturated calomel electrode. This is the average of seven independent determinations, with varying amounts of hydrogen and carbon dioxide.

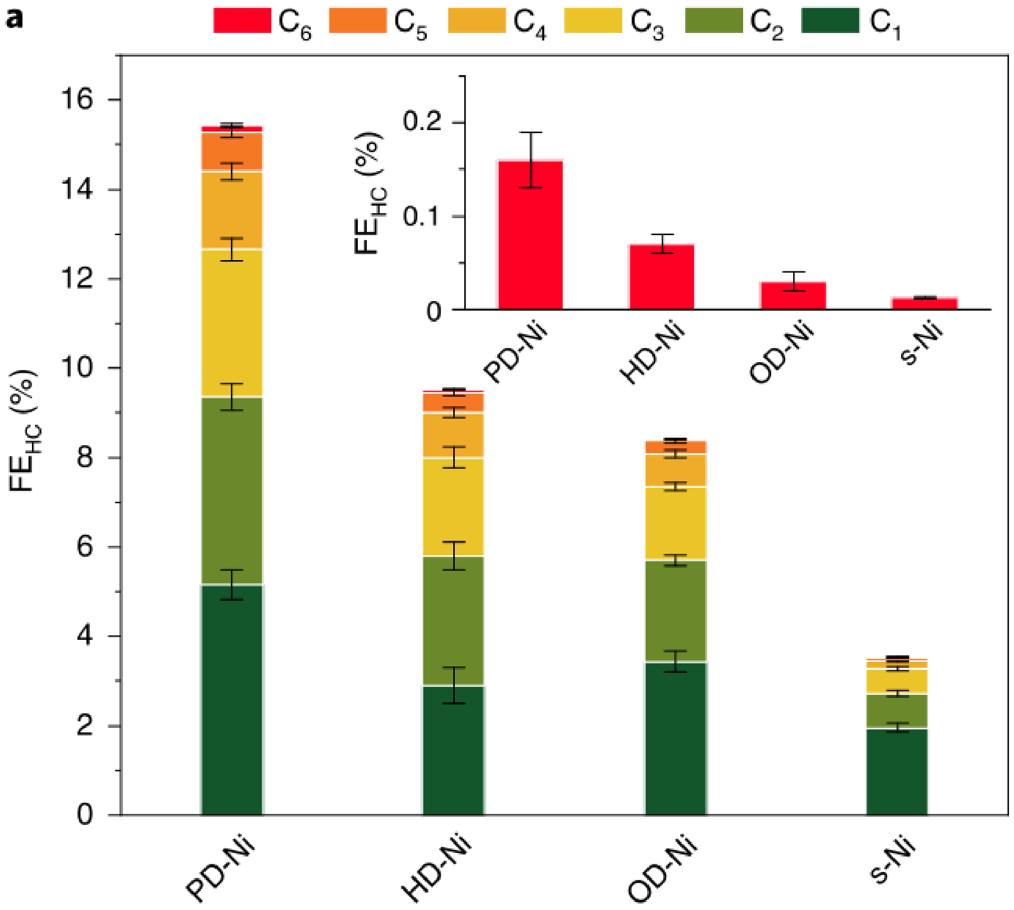
Van Rysselberghe, P.; Alkire, G. J.
J. Am. Chem. Soc. **1944**, *66*, 1801.

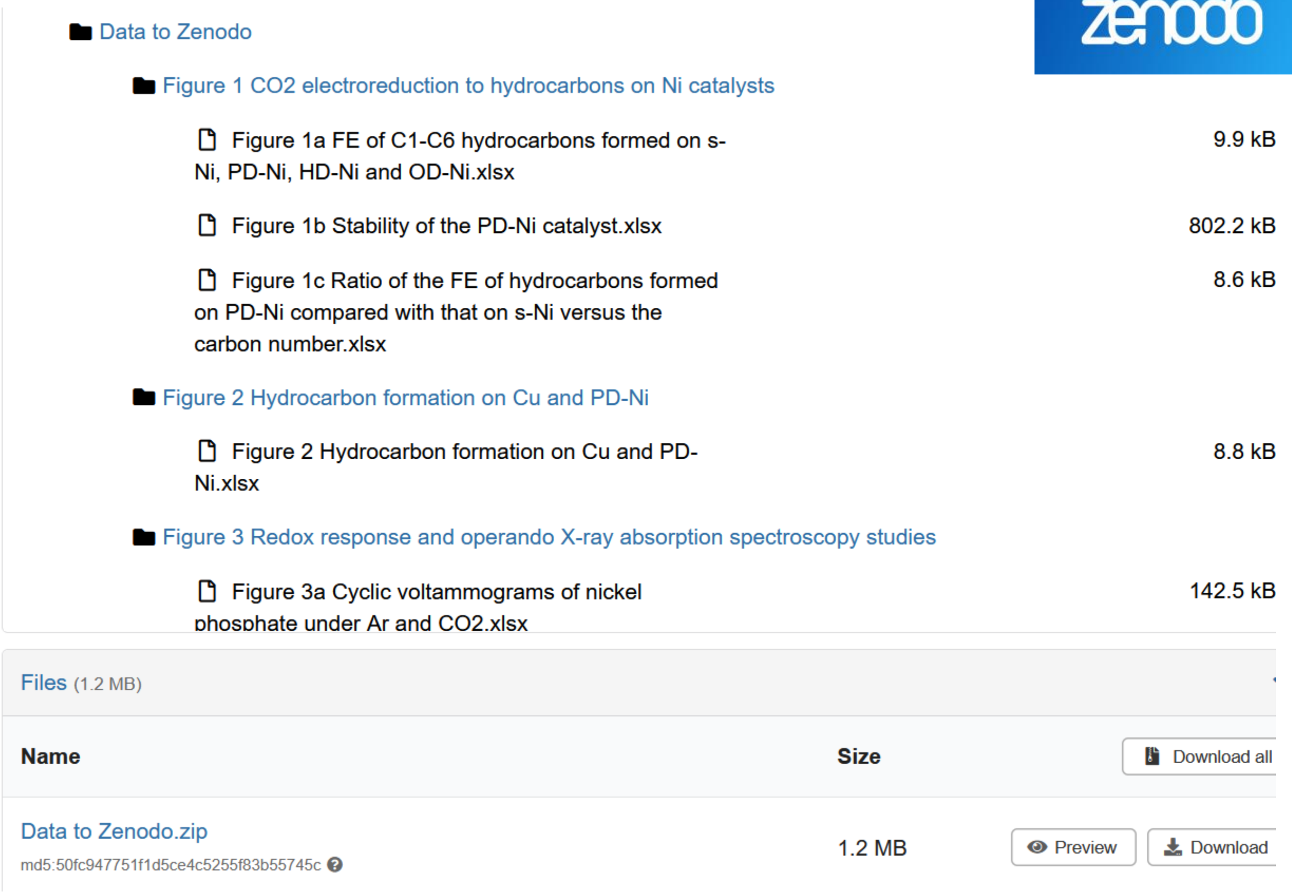


Search on Scopus database using keywords “Electrochemical CO_2 reduction”.
Scopus, https://www.scopus.com, online, accessed on 27/02/2025.

The need for FAIR protocols

Findability / **A**ccessibility / **I**nteroperability / **R**eusability

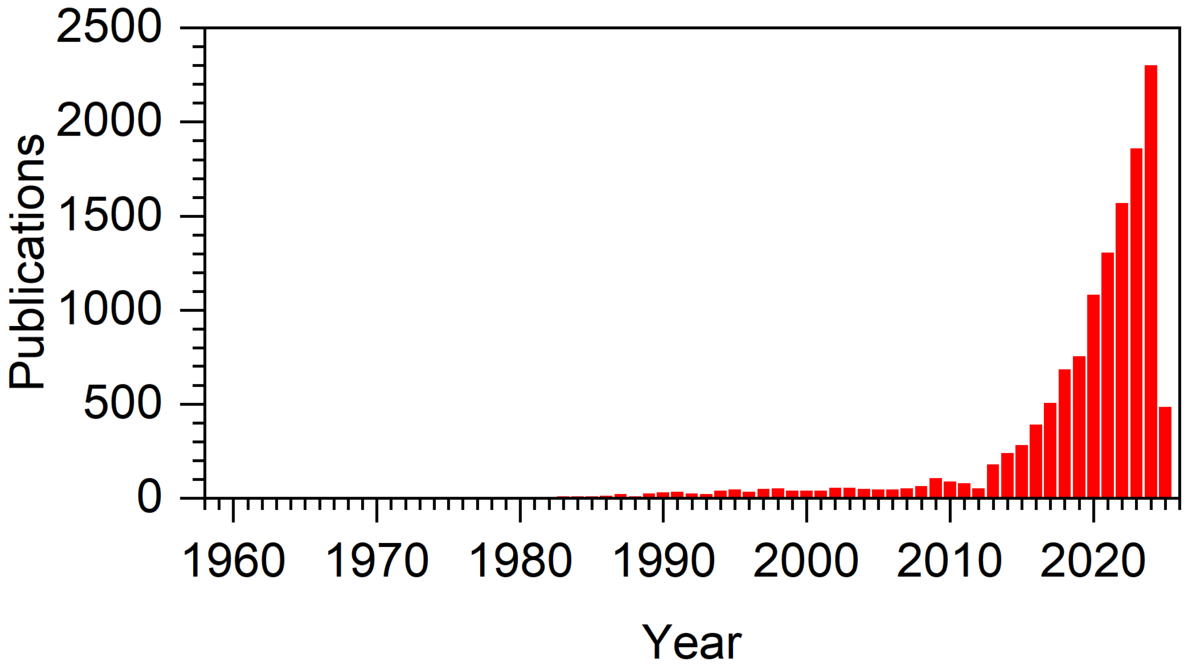




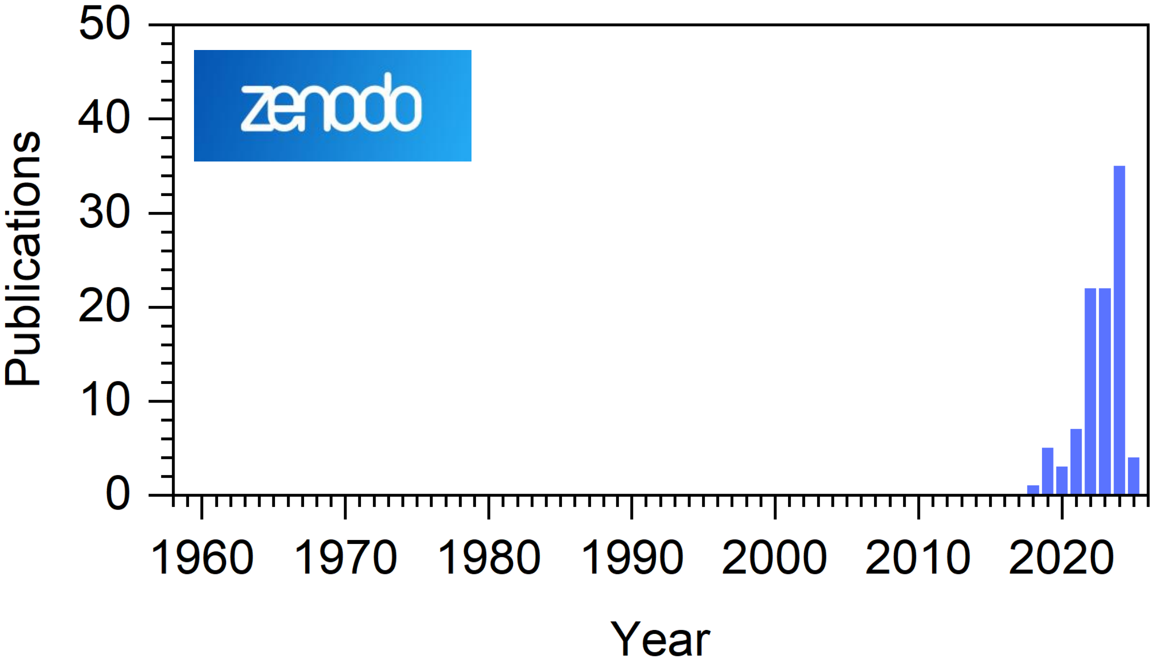
Zhou, Y. *et al. Nat. Catal.* **2022**, *5*, 545–554. https://doi.org/10.1038/s41929-022-00803-5.
ZENODO repository, https://doi.org/10.5281/zenodo.6331376, online, accessed on 24/09/2025.

The limit of current repositories

Keywords:
Electrochemical CO_2 reduction

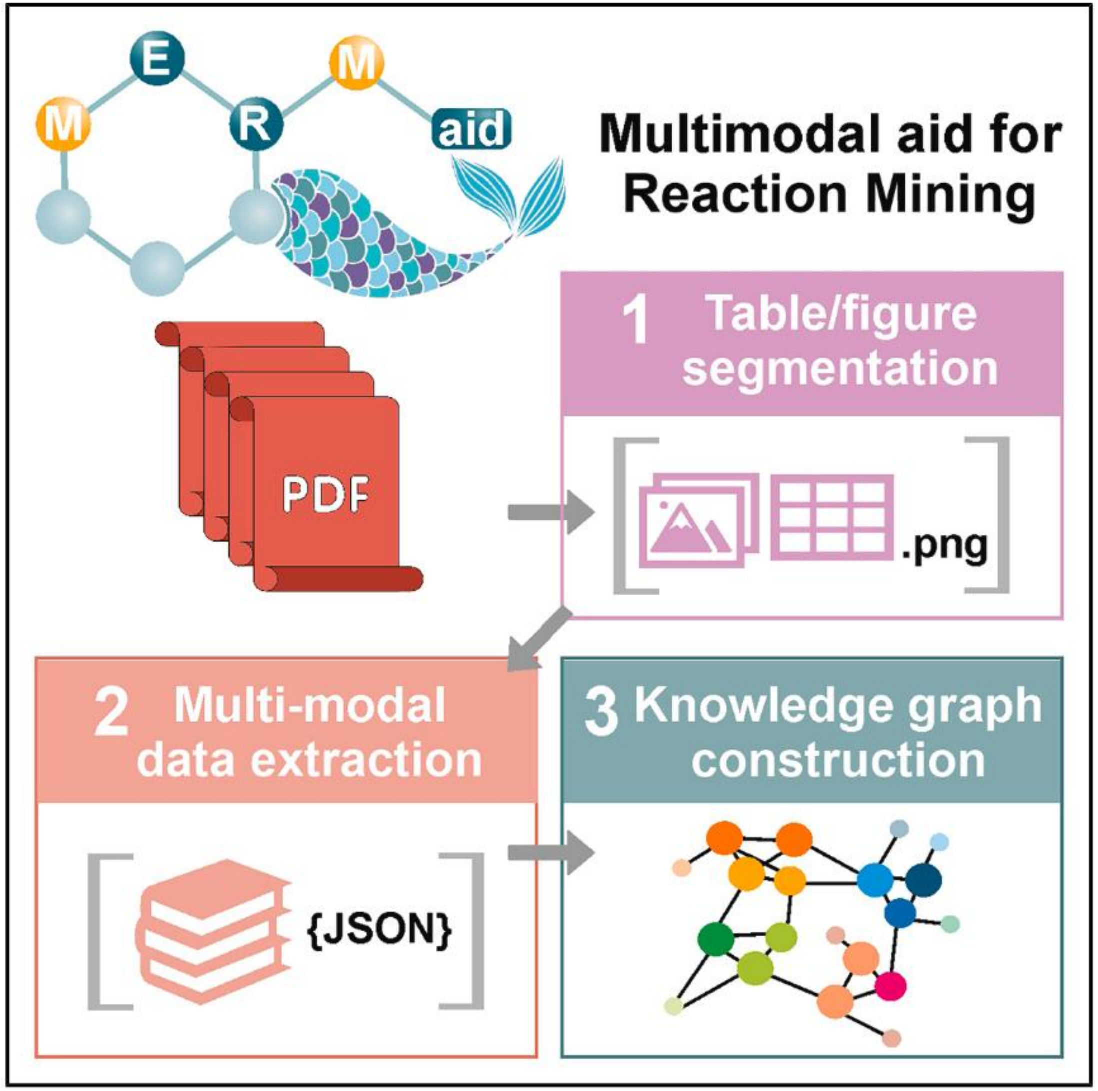


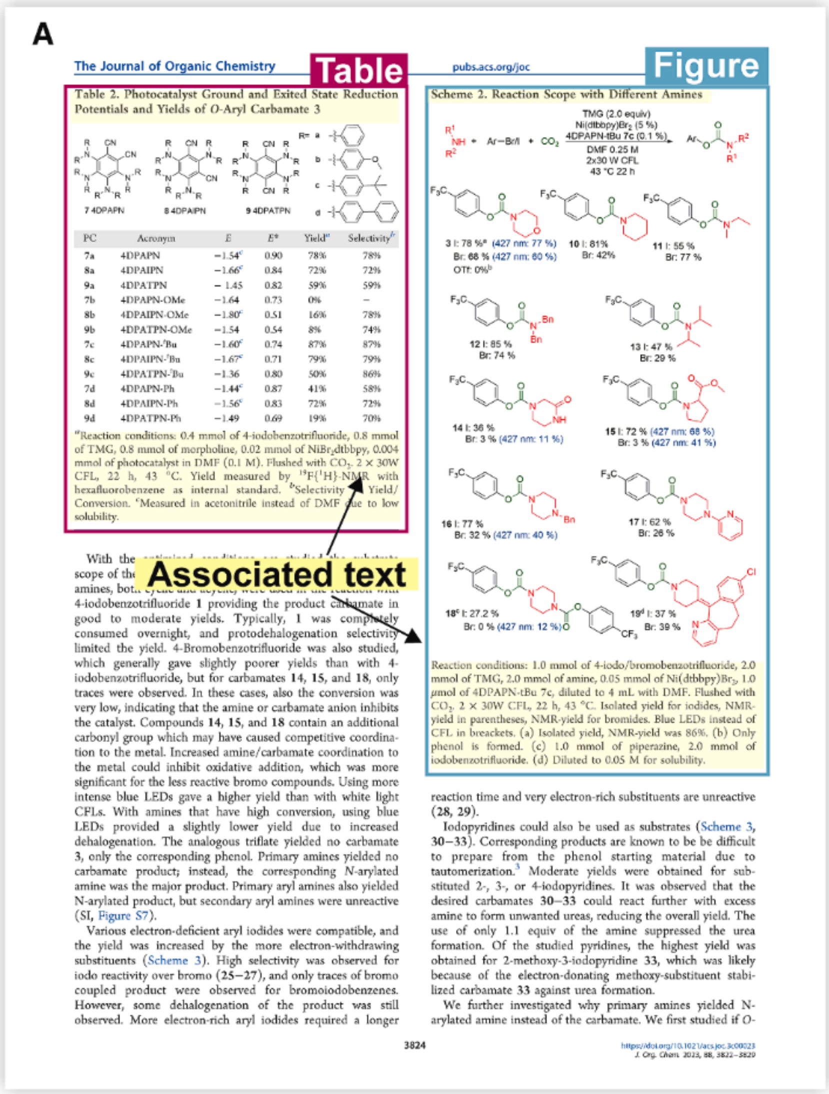
Keywords:
Electrochemical CO_2 reduction, Zenodo



Zenodo Platform, https://zenodo.org, online, accessed on 27/02/2025.
Scopus, https://www.scopus.com, online, accessed on 27/02/2025.

AI-based solution: MERMaid





Leong, S. X.; Pablo-García, S.; Wong, B.; Aspuru-Guzik, A. *Matter* **2025**, *8*, 102331. https://doi.org/10.1016/j.matt.2025.102331.

The SuPERCO2 concept

Embargo

Data Production

Storage

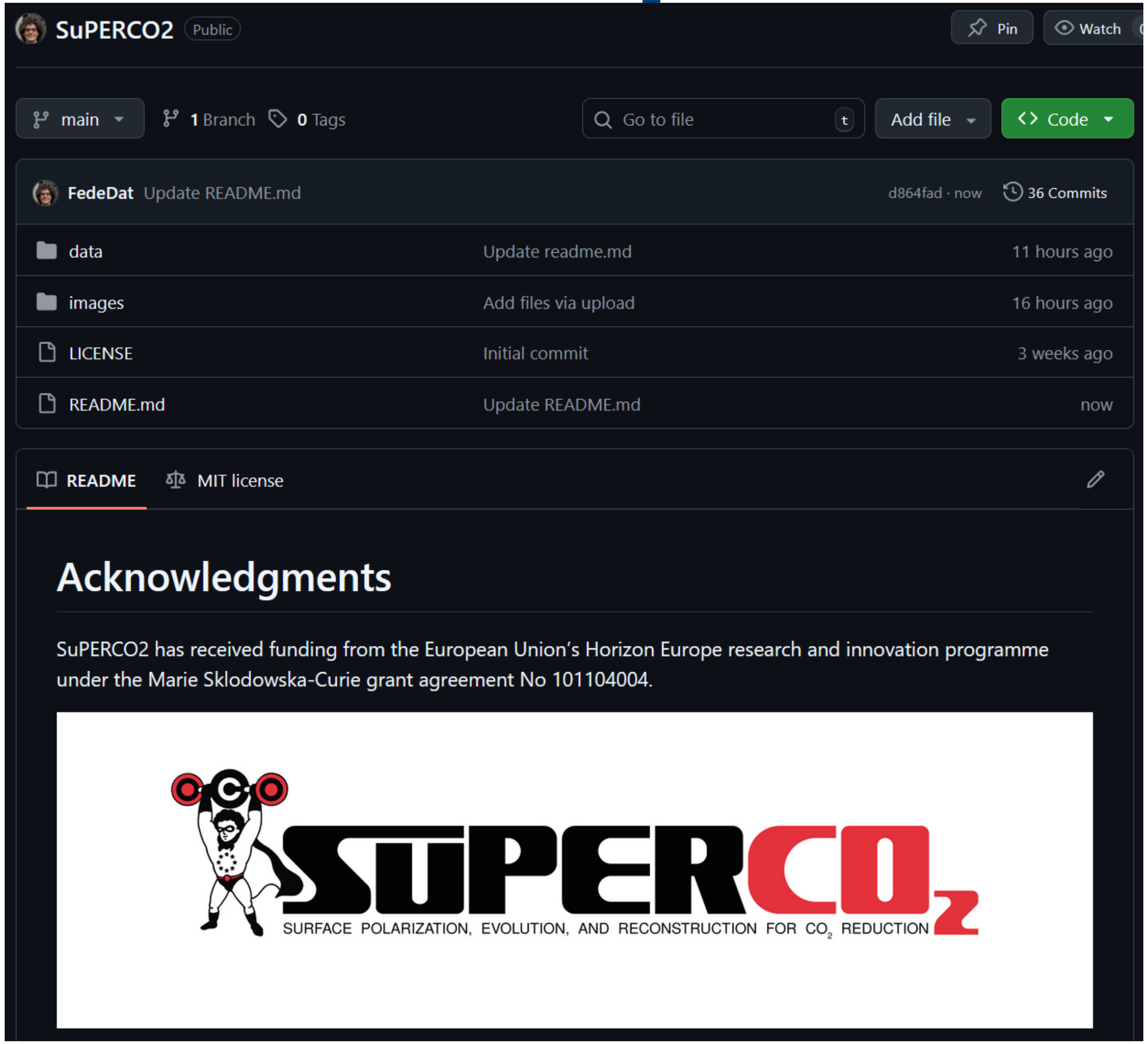
Raw Data

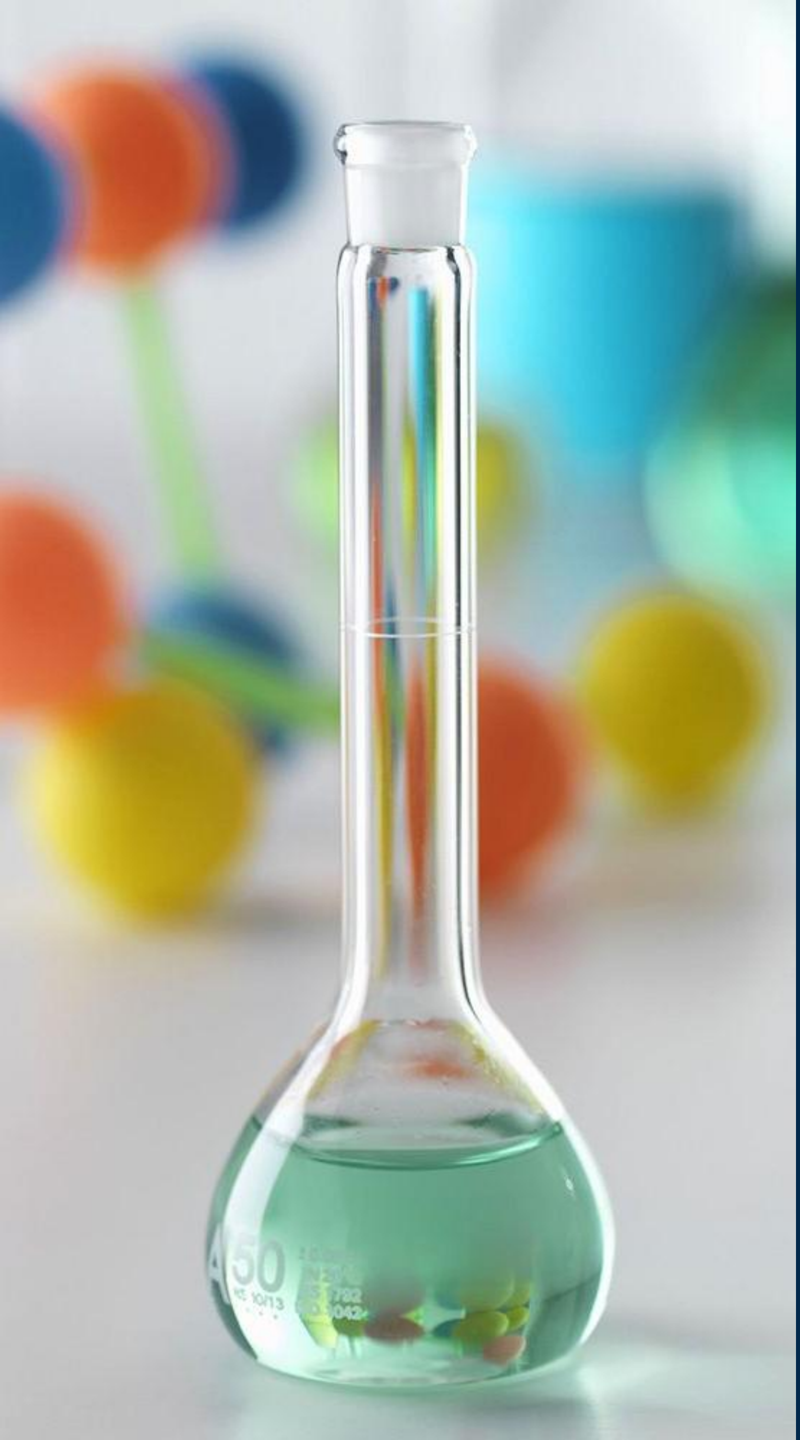
Data Analysis

Analysed Data

Publication

Lift embargo





Synthesis

Repository: github.com/FedeDat/SuPERCO2

item: data/CuO/synthesis

Internal logbook

Precursors

1	Precursor	CAS number	C (M)	C (mol)	V (mL)	m (g)	Molar mass (g/mol)
2	CuCl2 2H2O	10125-13-0	0.02	0.00	250.00	0.60	134.45
3	NaOH	1310-73-2	6.08	0.30	50.00	12.17	40.00
4	milliQ		55.50	13.88	250.00	249.96	18.02

Protocol

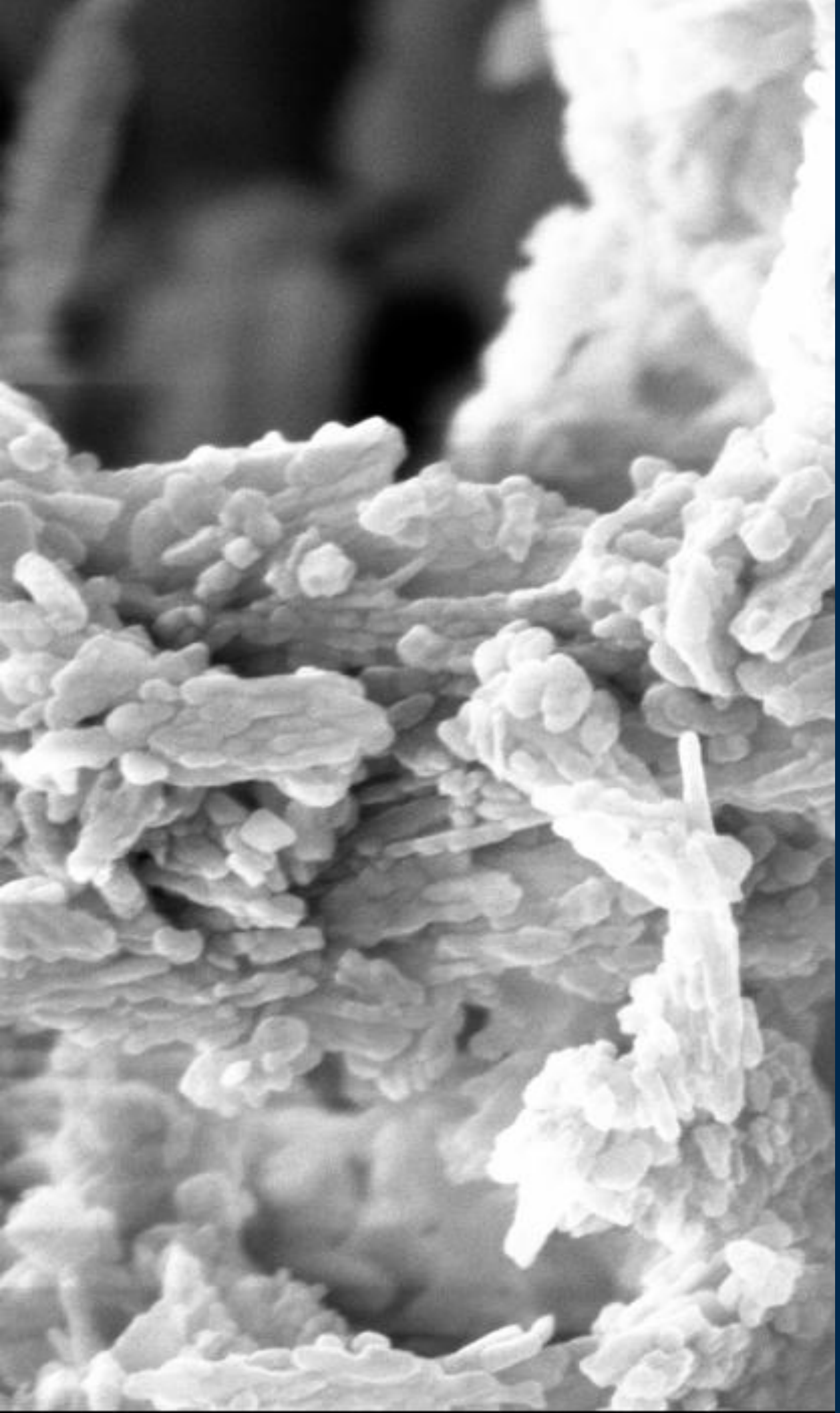
Equipment

- A Peristaltic Pump was used to control the flow rate during addition of the sodium hydroxide solutions.
- Magnetic stirrers were essential for ensuring uniform mixing of the reactants, thus they were employed whenever a solution was involved.
- A centrifuge was necessary for separating the precipitated particles from the reaction mixture

Synthesis procedure

Synthesis carried out on 03/07/2024.

The synthesis of CuO was a simple water-based precipitation, followed by calcination (Table 1). 250 mL of milliQ water were added to 600 mg of copper chloride (CuCl2··2H2O) under vigorous magnetic stirring to achieve a 20 mM solution. Then a solution of 6 M NaOH was formed by mixing 12.1674 g of NaOH into a 50 mL volumetric flask. After this, half the NaOH solution (25 mL) was added to the copper chloride solution via the peristaltic pump with a fixed flow rate of 25 mL per minute. As soon as NaOH was inserted, a light blue copper hydroxide precipitate appeared (Figure 7). The precipitate was centrifuged at 5000 rpm and cleaned with milliQ water. Four additional cleaning/centrifugation cycles were carried out, where the solvent was promptly removed. Then the resulting precipitate was transferred to a standard oven at 200 ºC for 2 hours where the hydroxide decomposed to CuO.



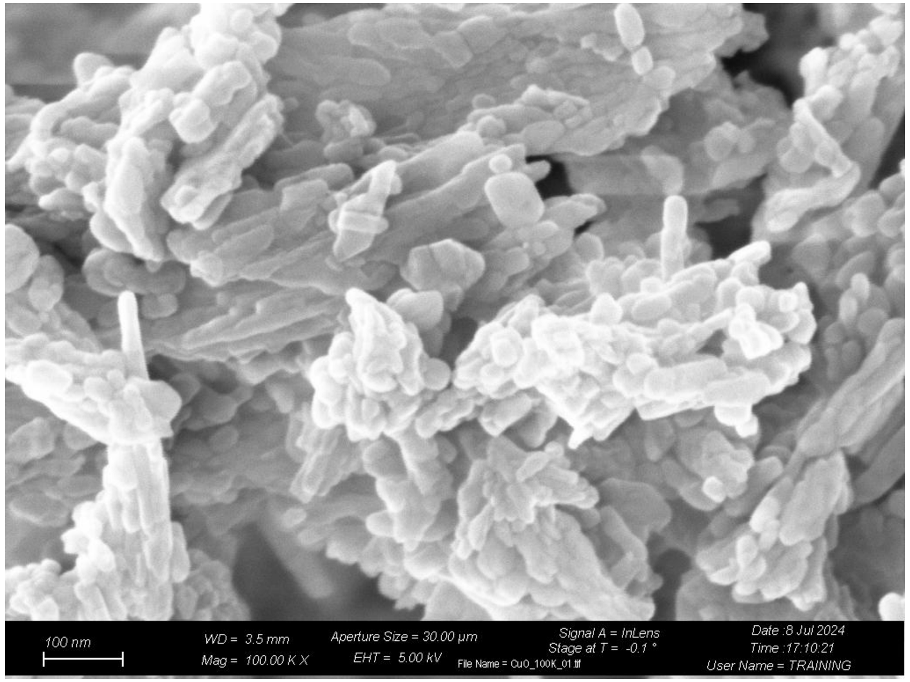
Characterization

Repository: github.com/FedeDat/SuPERCO2

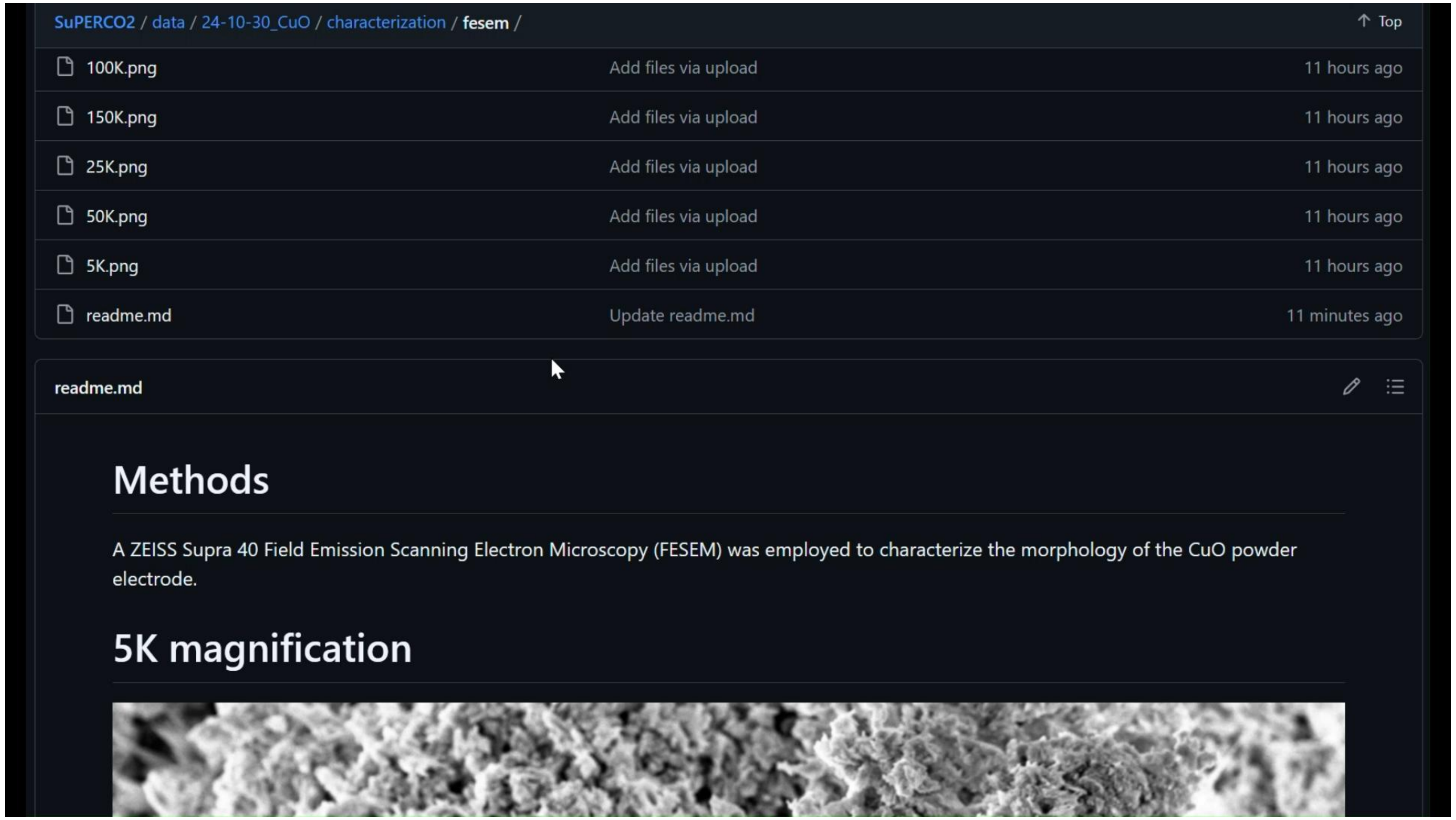
item: data/24-10-30_CuO/characterization

Scanning Electron Microscopy

Post-processing



Data analysis & Visualization



Energy Dispersive X-ray

Post-processing

FedeDat Add files via upload

Preview Code Blame 4 lines

Search this file

1	Cu	Fe	O	C	Na	Cl
2	42.59		57.41			
3	42.77		57.23			
4	41.37		58.63			

Data analysis & Visualization

```python
def cm_to_inch(cm):
    inch=float(cm/2.54)
    return inch

def AgCl_to_RHE(V_AgCl,pH,ref):
    if ref == "Ag/AgCl":
        V_RHE=+0.197+V_AgCl+0.059*pH
        return V_RHE

# Read the content of the file

url_EDX = "https://raw.githubusercontent.com/FedeDat/SuPERCO2/main/data/24-10-30_CuO/characterization/EDX.csv"

data_EDX = pd.read_csv(url_EDX, usecols=lambda column: pd.notnull(column))
data_EDX.dropna(axis=1, how='all', inplace=True)

#Calculate ratio between metal and oxygen

data_EDX[''+str(data_EDX.columns[0])+'/'+str(data_EDX.columns[1])+'']=data_EDX[data_EDX.columns[0]]/data_EDX[data_EDX.column

data_EDX.index=list(range(1, len(data_EDX)+1))

ax1 = data_EDX.iloc[:,:-1].plot(kind='bar', stacked=True, figsize=(cm_to_inch(10), cm_to_inch(8)))
plt.legend(loc='upper center')

ax2 = ax1.twinx()  # Create a second y-axis
ax2.plot(data_EDX.index-1, data_EDX[data_EDX.columns[-1]], linestyle='None', marker='o', markersize=8, markerfacecolor='red'

# Adding titles and labels
ax1.set_xticklabels(list(range(1, len(data_EDX)+1)), rotation=0, ha='right')
```

X-ray Diffraction

Post-processing

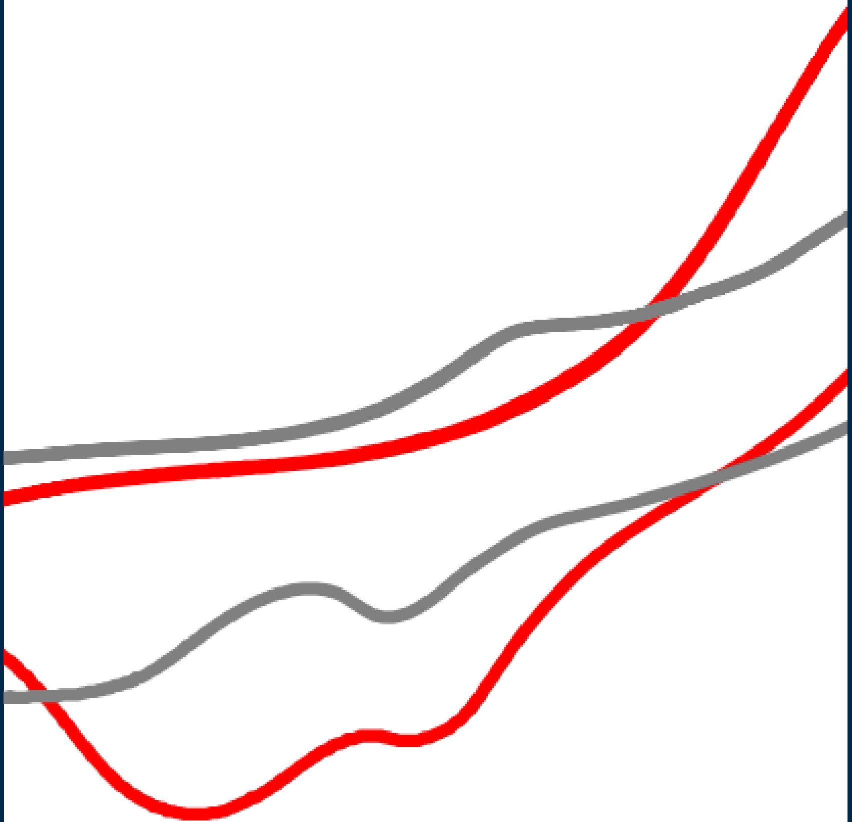
SuPERCO2 / data / 24-10-30_CuO / characterization / XRD.csv

Preview | Code | Blame   2694 lines (2694 loc) · 46 KB

Angle	Intensity
20.01513028	862
20.04139085	848
20.06765141	881
20.09391198	856
20.12017254	853
20.14643311	891
20.17269367	876

Data analysis & Visualization

```
def AgCl_to_RHE(V_AgCl,pH,ref):
    if ref == "Ag/AgCl":
        V_RHE=+0.197+V_AgCl+0.059*pH
        return V_RHE

url_XRD = "https://raw.githubusercontent.com/FedeDat/SuPERCO2/main/data/24-10-30_CuO/characterization/XRD.csv"

data_XRD = pd.read_csv(url_XRD, header=None, usecols=[0, 1], names=['Angle', 'Intensity'])

k_XRD = float(data_XRD[data_XRD.apply(lambda row: row.astype(str).str.contains('K-Alpha1 wavelength')).any(axis=1)]['Intensit

n_XRD = int(data_XRD[data_XRD.apply(lambda row: row.astype(str).str.contains('No. of points')).any(axis=1)]['Intensity'])

data_XRD_sl = data_XRD.iloc[(data_XRD[data_XRD.apply(lambda row: row.astype(str).str.contains('Angle')).any(axis=1)].index[0]

data_XRD_sl = data_XRD_sl.astype(float)

data_XRD_sl['Intensity'] = data_XRD_sl['Intensity'] - np.min(data_XRD_sl['Intensity'])

data_XRD_sl['Intensity']=data_XRD_sl['Intensity']/np.max(data_XRD_sl['Intensity'])

data_XRD_sl['Intensity_savgol'] = savgol_filter(data_XRD_sl['Intensity'], window_length=10, polyorder=1)

k_XRD = float(data_XRD[data_XRD.apply(lambda row: row.astype(str).str.contains('K-Alpha1 wavelength')).any(axis=1)]['Intensit

n_XRD = int(data_XRD[data_XRD.apply(lambda row: row.astype(str).str.contains('No. of points')).any(axis=1)]['Intensity'])
```



Electrochemical testing

Repository: github.com/FedeDat/SuPERCO2

item: data/CuO/electrochemistry

Open Circuit Potential

Post-processing

SuPERCO2 / data / 24-10-30_CuO / EC / OCV.csv

FedeDat Add files via upload

Preview Code Blame 548 lines (548 loc)

Search this file

1	pH	6.8
2	Ref	Ag/AgCl
3		
4	t (min)	Ewe (V)
5	0.00E+00	-2.14E-01

Data analysis & Visualization

```python
# Read the content of the file

url_OCV = "https://raw.githubusercontent.com/FedeDat/SuPERCO2/main/data/24-10-30_CuO/EC/OCV.csv"

data_OCV = pd.read_csv(url_OCV, header=None, names=['time', 'V'])

pH_OCV=float(data_OCV['V'][0])
ref_OCV=str(data_OCV['V'][1])

data_OCV=data_OCV[4:]

data_OCV=data_OCV.astype(float)

data_OCV['V']=AgCl_to_RHE(data_OCV['V'],6.8,ref_OCV)

plt.figure(figsize=(cm_to_inch(12), cm_to_inch(8)))

plt.plot(data_OCV['time'],data_OCV['V'], )

plt.title('Open circuit potential')

plt.xlabel(r"$t$ (min)")
plt.ylabel(r"$V$ (vs RHE)")

plt.ylim(min(np.min(data_OCV['V']),0.5*np.mean(data_OCV['V'])),max(np.max(data_OCV['V']),1.5*np.mean(data_OCV['V'])))

plt.savefig('OCV.png', format='png', dpi=300, transparent=True, bbox_inches='tight')

#plt.close()
```

Cyclic voltammetry

Post-processing

SuPERCO2 / data / 24-10-30_CuO / EC / CV-CO2.csv

FedeDat Add files via upload

Preview Code Blame 1810 lines (1810 loc) ·

Search this file

1	pH	6.8
2	Ref	Ag/AgCl
3		
4	Ewe (V)	j (mA/cm2)
5	-1.45E+00	-8.35E+00

Data analysis & Visualization

```
data_CV_CO2['V']=AgCl_to_RHE(data_CV_CO2['V'],6.8,ref_CV_CO2)

url_CV_N2 = "https://raw.githubusercontent.com/FedeDat/SuPERCO2/main/data/24-10-30_CuO/EC/CV-N2.csv"
data_CV_N2 = pd.read_csv(url_CV_N2, header=None, names=['V', 'j'])

pH_CV_N2=float(data_CV_N2['j'][0])
ref_CV_N2=str(data_CV_N2['j'][1])

data_CV_N2=data_CV_N2[4:]

data_CV_N2=data_CV_N2.astype(float)

data_CV_N2['V']=AgCl_to_RHE(data_CV_N2['V'],6.8,ref_CV_N2)

plt.figure(figsize=(cm_to_inch(12), cm_to_inch(12)))

plt.plot(data_CV_CO2['V'],data_CV_CO2['j'], label=r"CO$_2$ saturated",color='red')
plt.plot(data_CV_N2['V'],data_CV_N2['j'], label=r"N$_2$ saturated",color='gray')

plt.title('Cyclic voltammetry')
plt.legend(loc='best')

plt.xlabel(r"$V$ (vs RHE)")

plt.ylabel(r"$j$ (mA/cm$^2$)")

plt.savefig('CV.png', format='png', dpi=300, transparent=True, bbox_inches='tight')

#plt.close()
```

alculation of CO_2 reduction activity and selectivity

```
# Analyse Faradaic Efficiency
```

Chronoamperometry

Post-processing (CA)

SuPERCO2 / data / 24-10-30_CuO / EC / CA1.csv

FedeDat Add files via upload

Preview Code Blame 21125 lines (21125 l

Search this file

1	pH	6.8
2	Ref	Ag/AgCl
3	V	-1.199
4	Flow Rate (NmL/min)	20
5	Type	CA
6		
7	t (s)	j (mA/cm2)
8	2.63E+00	-2.43E-05

Post-processing (GC)

SuPERCO2 / data / 24-10-30_CuO / EC / GC1.csv

FedeDat Add files via upload

Preview Code Blame 11 lines (11 loc) · 392 Bytes

Search this file

1	H2	O2	N2	CH4	CO	CO2	C2H4
2	0	0	0.938709	0.00071317	0	0	0
3	0.08128675	0	0.94220475	0	0	0	0
4	0.15007389	0	0.93674202	0	0	0	0
5	0.14496378	0	0.93663998	0	0	0	0
6	0.14065497	0	0.92155004	0	0	0	0
7	0.14463469	0	0.91517259	0	0	0	0
8	0.14796505	0	0.91493298	0	0	0	0

Activity & Selectivity

Data analysis & Visualization

Work in progress for liquid products

Calculation of CO_2 reduction activity and selectivity

```
# Analyse Faradaic Efficiency

# GitHub API URL for the folder
api_url = "https://api.github.com/repos/FedeDat/SuPERCO2/contents/data/24-10-30_CuO/EC"

# Get the file listing
response = requests.get(api_url)
files = response.json()

metadata_EC = pd.DataFrame(columns=['pH', 'ref', 'V'])
anl_EC = pd.DataFrame(columns=['V_RHE','Flow Rate','Mode','Average j', 'Q (mC)'])

data = pd.DataFrame()

n1=0

plt.figure(figsize=(cm_to_inch(18), cm_to_inch(12)))
```

Chronopotentiometry

Post-processing (CP)

Preview | Code | Blame 918 lines (918 loc) · 38.8 KB

Search this file

1	**Area (cm2)**	**1.33**		
2	Electrolyte	KOH		
3	Conc (M)	1		
4	Loading (mg/cm2)	0.6		
5	pH initial vs final	14	13.73	
6	ZIR (Ohm)	4.945	4.801	
7	Ref	Ag/AgCl		
8	V			
9	CO2 Flow Rate input vs output (mL/min)	10	8.7	
10	Electrolyte Flow Rate (mL/min)	1		
11	Type	CP		
12				
13	t (s)	i (mA)	Ewe (V)	Ecell (V)
14	29.99979924	0	-0.35689005	-0.12803969

Post-processing (GC, HPLC)

1	H2	O2	N2	CH4
2	33107.7722			131.4632
3	43991.6529			141.6516
4	52639.5361			148.6601
5	60080.1305			143.4467
6	66500.9825			141.7904
7	71986.6802			139.0178
8	71553.3711			0

1	HCOO-	AcO-
2	3.6034	0.0714
3		
4		
5		
6		
7		

The FAIR CO_2R problem

Open data is limited in CO_2R

Zenodo limits interoperability

AI mining on published data

The SuPERCO2 concept

Early data sharing

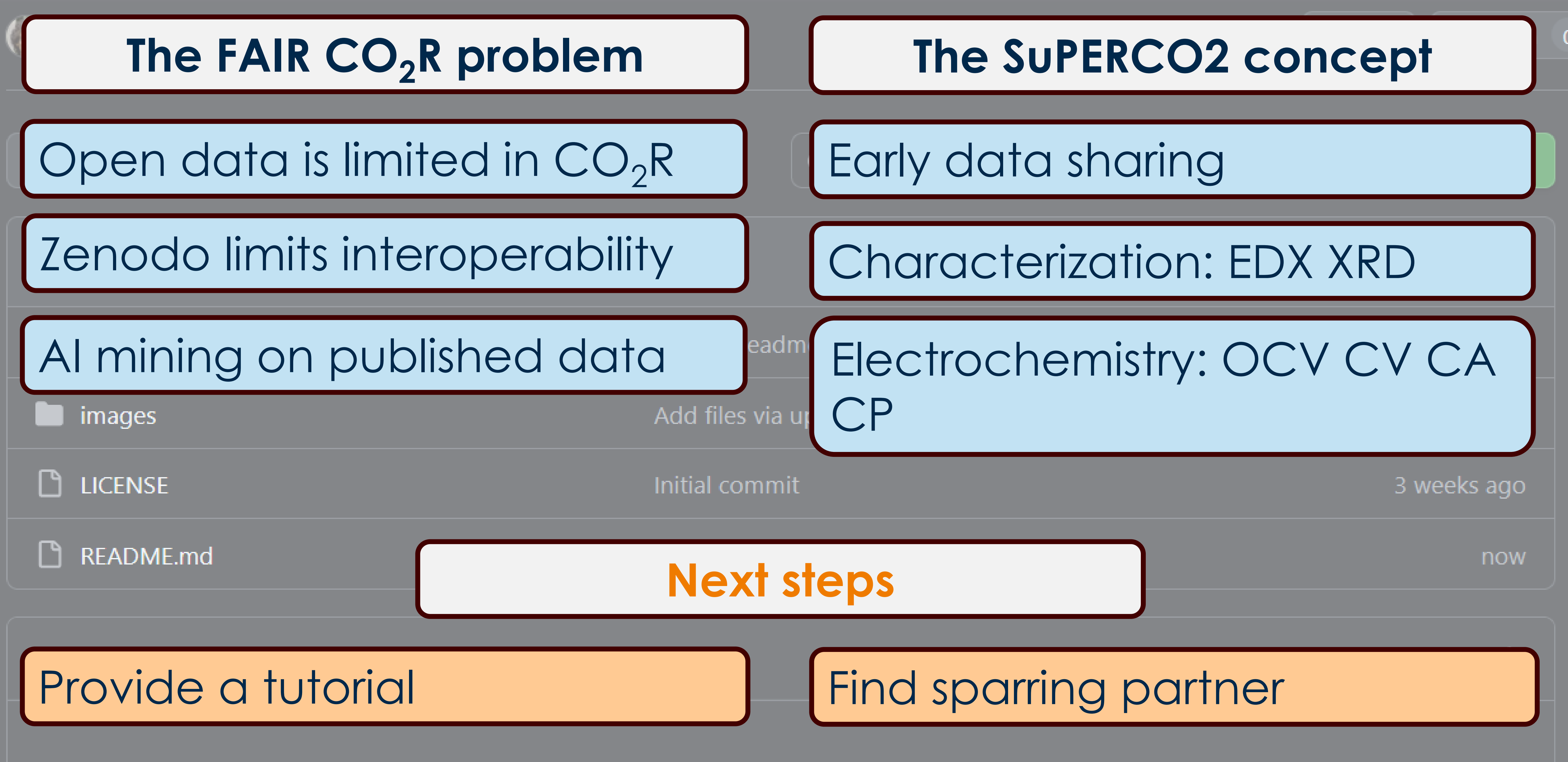
Characterization: EDX XRD

Electrochemistry: OCV CV CA CP

Next steps

Provide a tutorial

Find sparring partner



Let's try the power of SuPERCO2!

Politecnico di Torino

1859

Acknowledgements

Inspiration

M.Eng. Moisés Àlvarez (ICIQ)

ioChem-BD

Exp collaboration

M.Sc. Ali Zarei
(catalyst synthesis, electrochemical testing)

Prof. Simelys Hernández
(lab Access)

Politecnico di Torino 1859

DiSAT ECCELLENZA 2019 – 2027

Financial support

European Commission
Marie Skłodowska-Curie Actions
Research Fellowship Programme

SuPERCO2
SURFACE POLARIZATION, EVOLUTION, AND RECONSTRUCTION FOR CO_2 REDUCTION

SuPERCO2 has received funding from the European Union's Horizon Europe research and innovation programme under the Marie Sklodowska-Curie grant agreement No 101104004.

Thank you!
Questions or feedbacks?

Here or via email
(federico.dattila@polito.it)

Politecnico
di Torino