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

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Politecnico di Torino

SESSION 3 – (ELECTRO)CATALYSIS IN ENERGY CONVERSION & STORAGE

25/09/25, Belgrade, Serbia

The polytechnic of Turin

Located in Turin

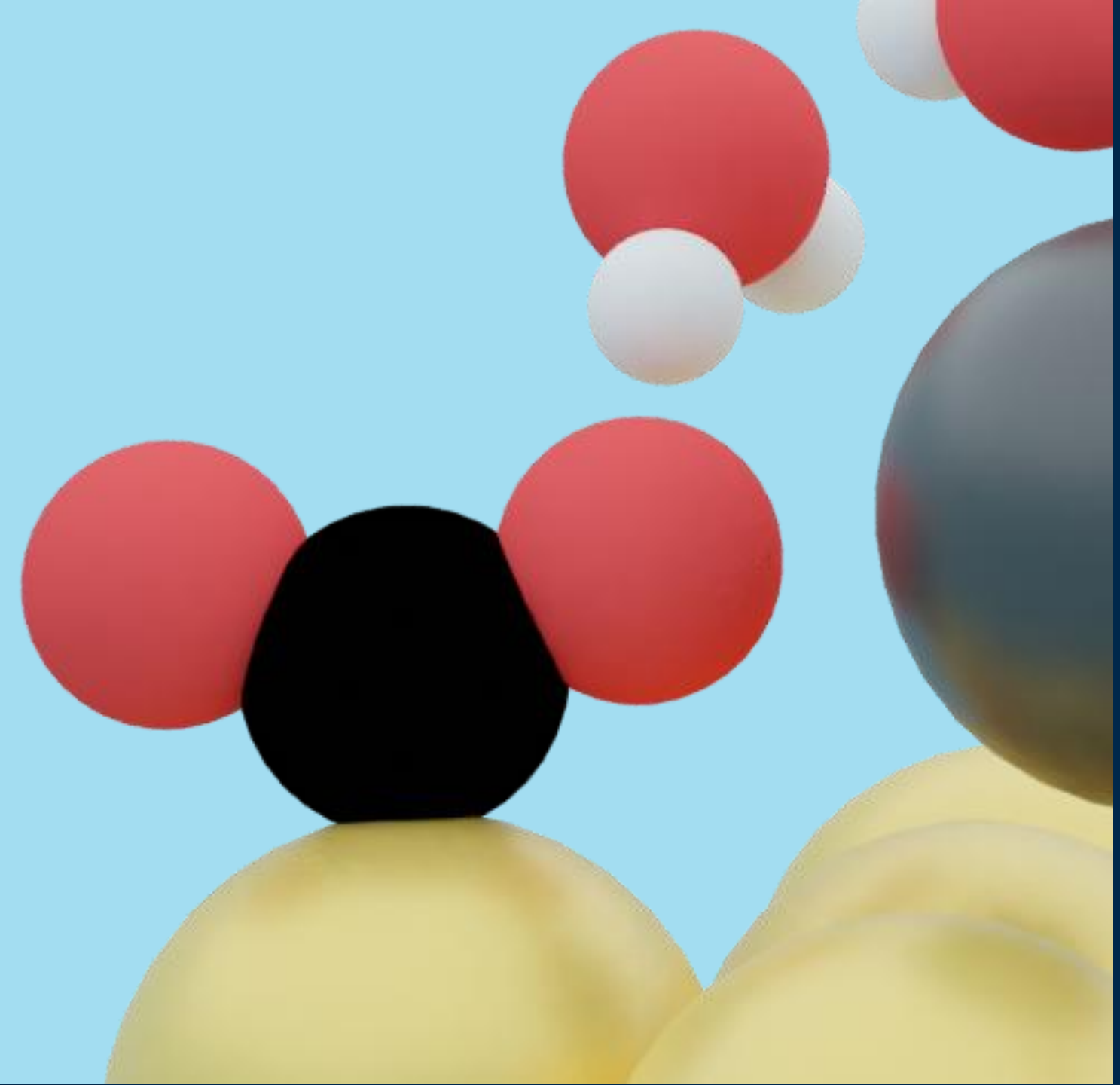
Technical university since 1859

Both experimental and computational groups working on electrocatalysis

1.5h flight Milan-Belgrade, then 2h bus

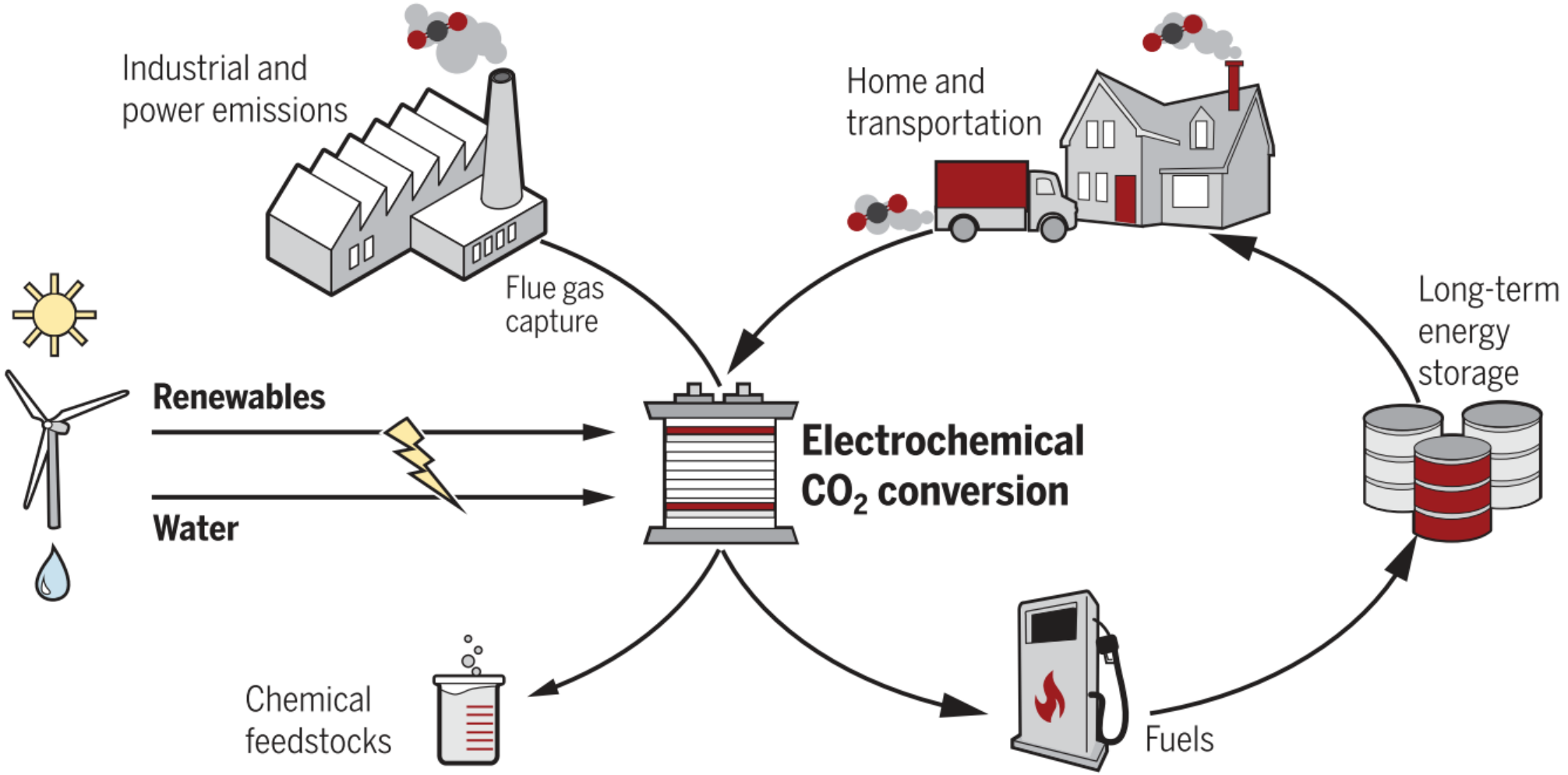
Politecnico di Torino
Dipartimento di Scienza Applicata e Tecnologia

DiSAT
ECCELLENZA 2019 – 2027



The FAIR problem of CO_2R

Electrochemical CO_2 reduction



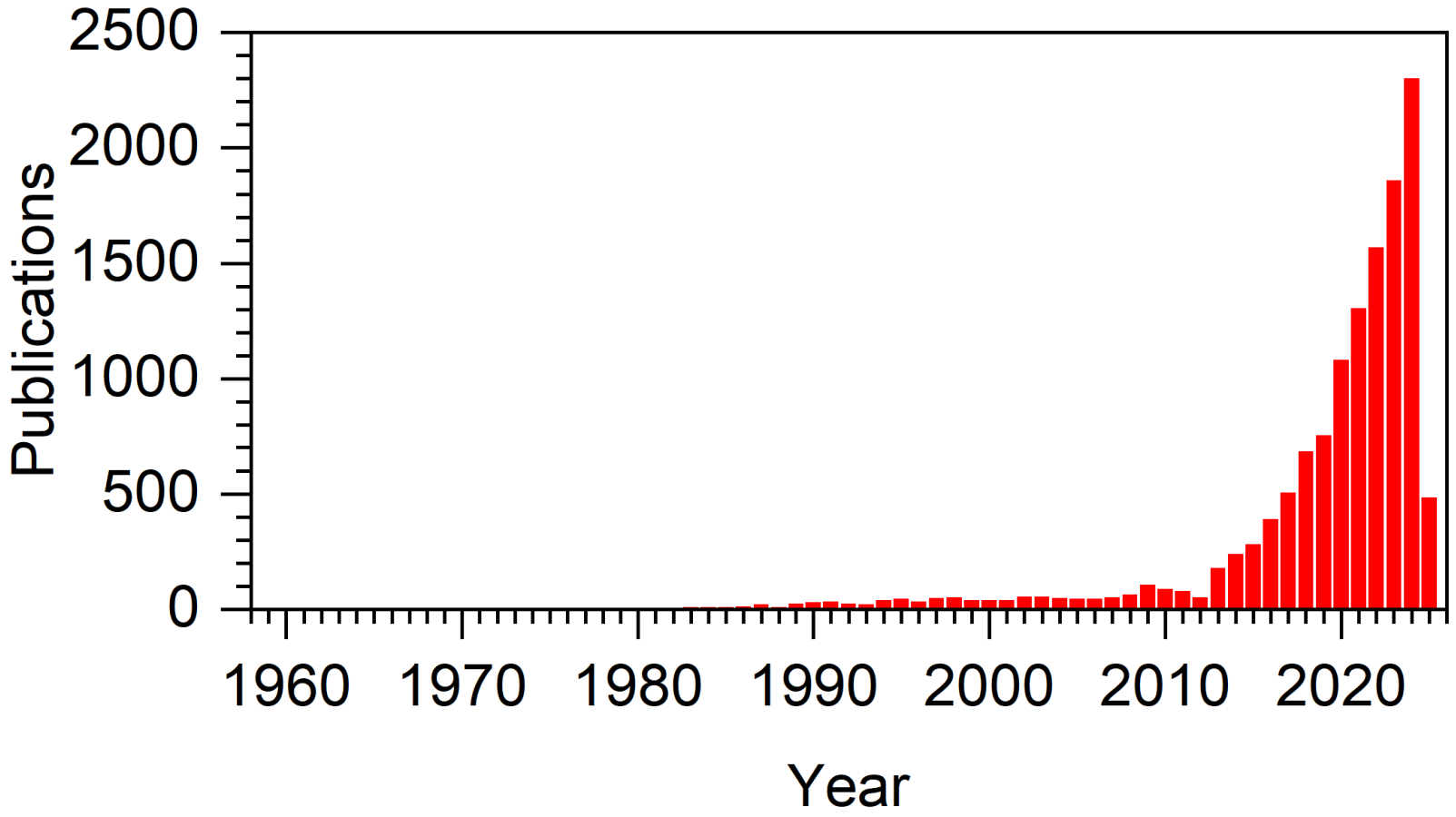
Publications on CO_2R

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.

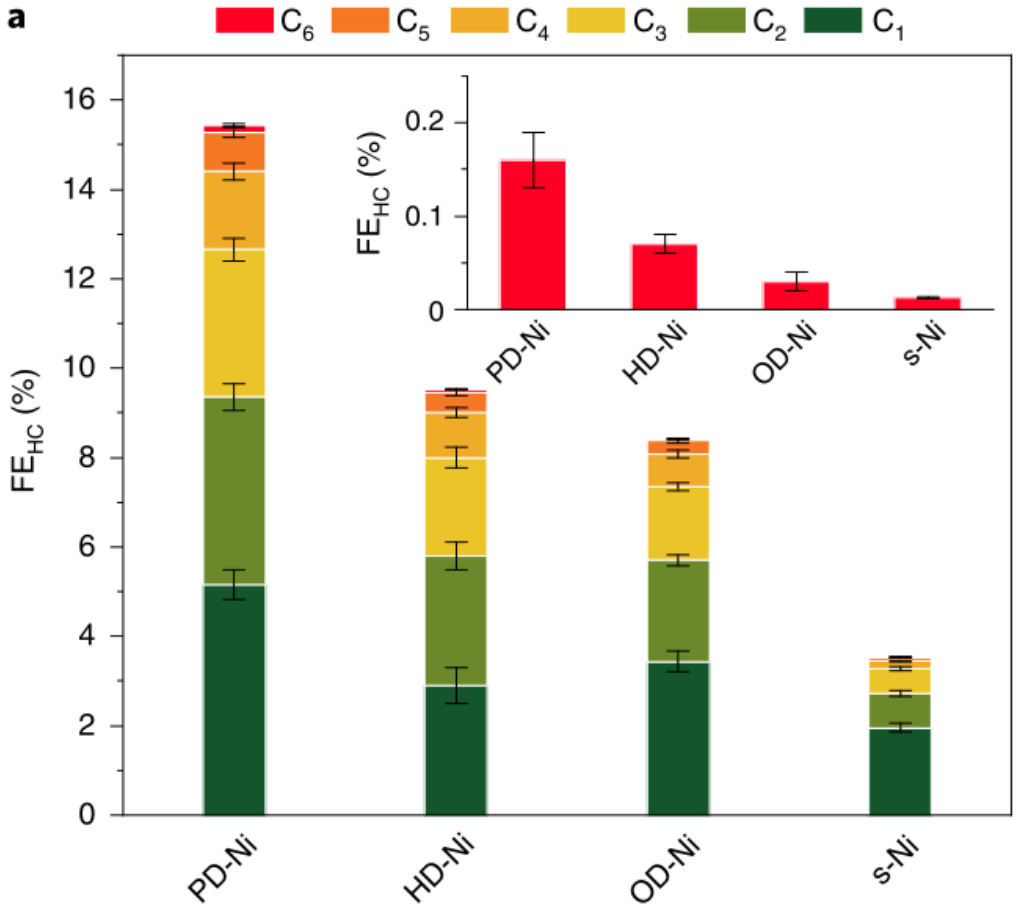
Van Rysselberghe, P.; Alkire, G. J.
J. Am. Chem. Soc. **1944**, 66, 1801.



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



zenodo

Data to Zenodo

Figure 1 CO2 electroreduction to hydrocarbons on Ni catalysts

Figure 1a FE of C1-C6 hydrocarbons formed on s-Ni, PD-Ni, HD-Ni and OD-Ni.xlsx	9.9 kB
Figure 1b Stability of the PD-Ni catalyst.xlsx	802.2 kB
Figure 1c Ratio of the FE of hydrocarbons formed on PD-Ni compared with that on s-Ni versus the carbon number.xlsx	8.6 kB

Figure 2 Hydrocarbon formation on Cu and PD-Ni

Figure 2 Hydrocarbon formation on Cu and PD-Ni.xlsx	8.8 kB

Figure 3 Redox response and operando X-ray absorption spectroscopy studies

Figure 3a Cyclic voltammograms of nickel phosphate under Ar and CO2.xlsx	142.5 kB

Files (1.2 MB)

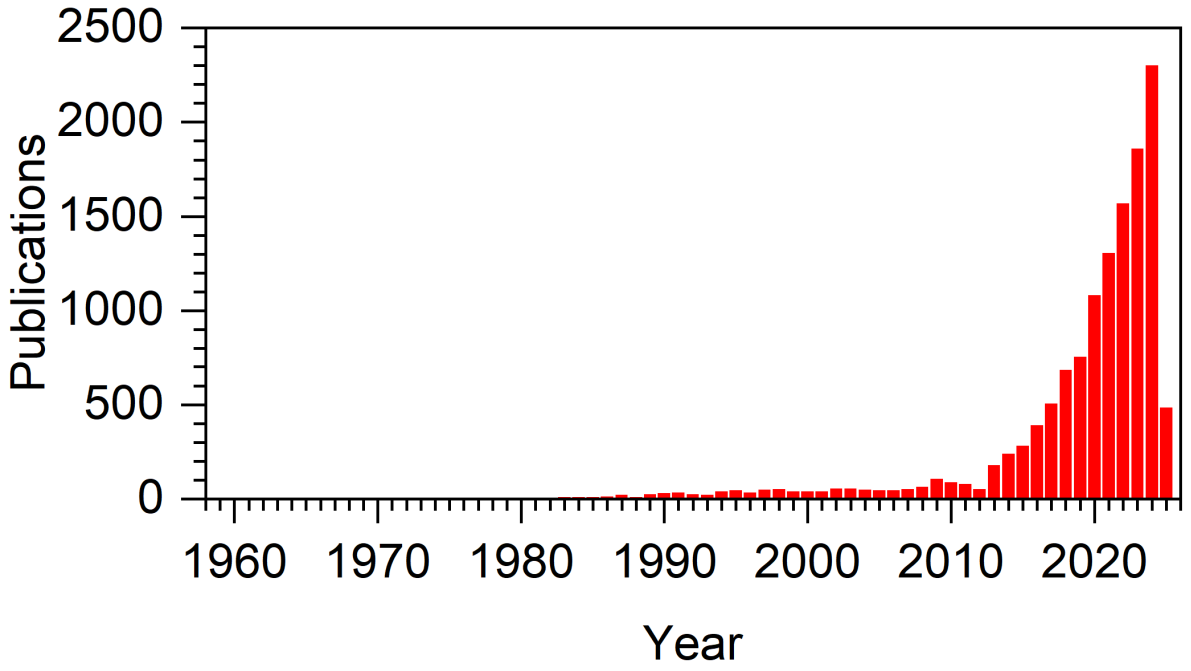
Name	Size	
Data to Zenodo.zip md5:50fc947751f1d5ce4c5255f83b55745c	1.2 MB	Preview Download

Download all

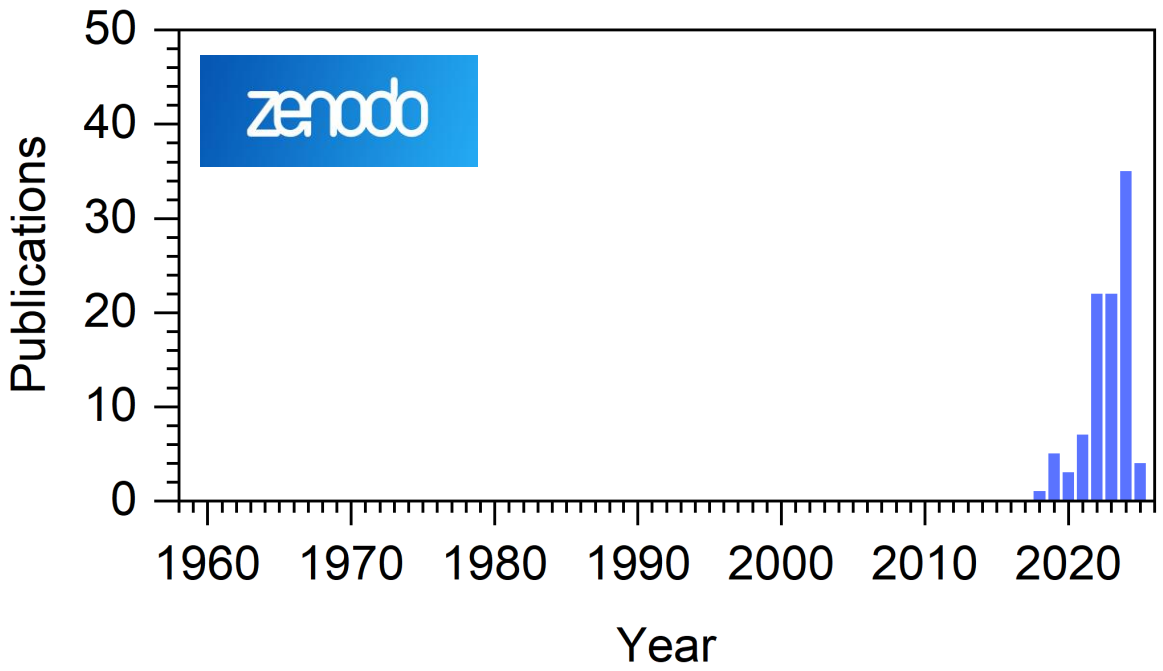
Zhou, Y. *et al. Nat. Catal.* **2022**, *5*, 545–554. https://doi.org/10.1038/s41929-022-00803-5.
ZENODO repository, https://doi.org/10.5281/zenodo.6331376, online, accessed on 24/09/2025.

The limit of current repositories

Keywords:
Electrochemical CO_2 reduction

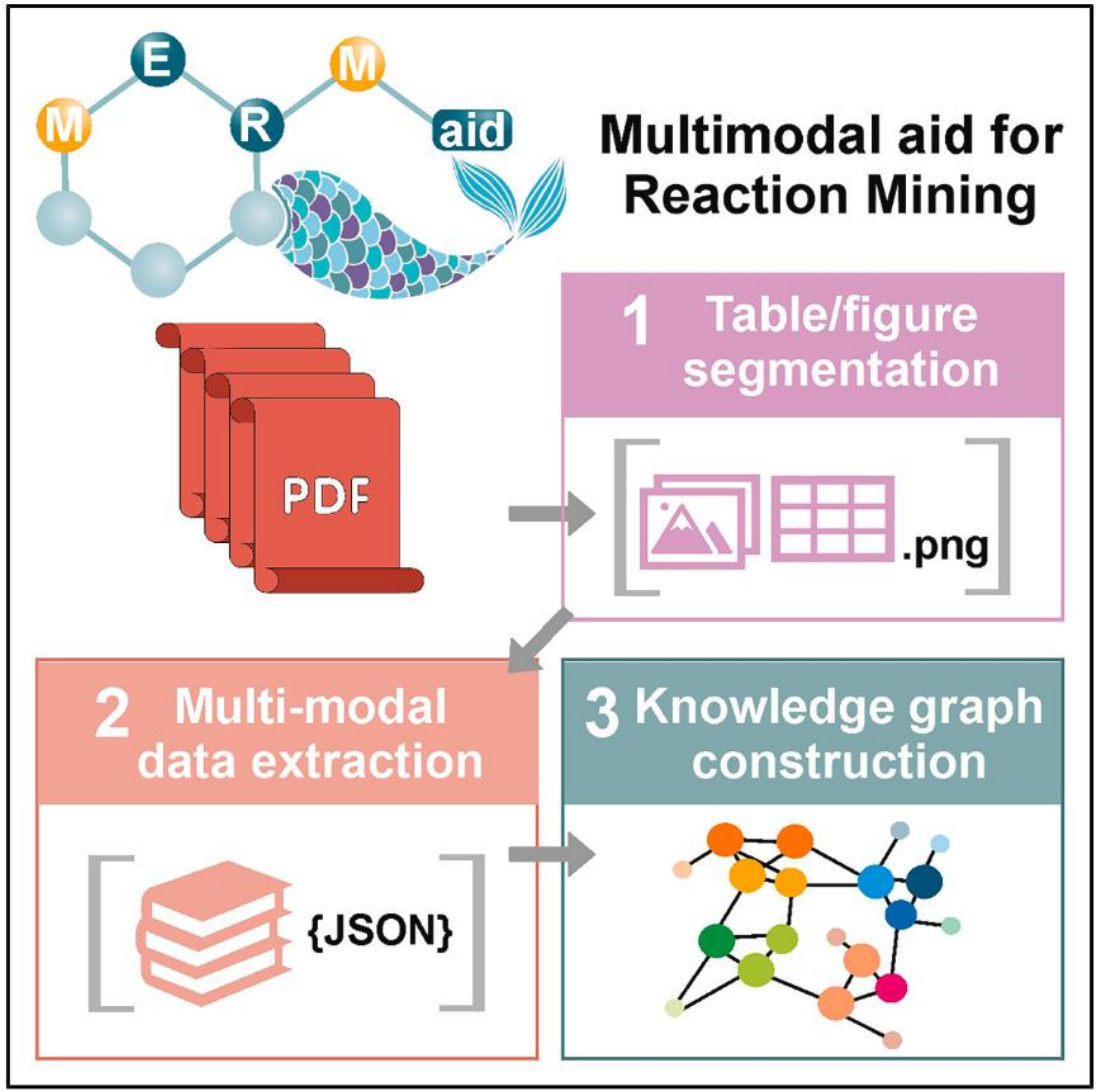


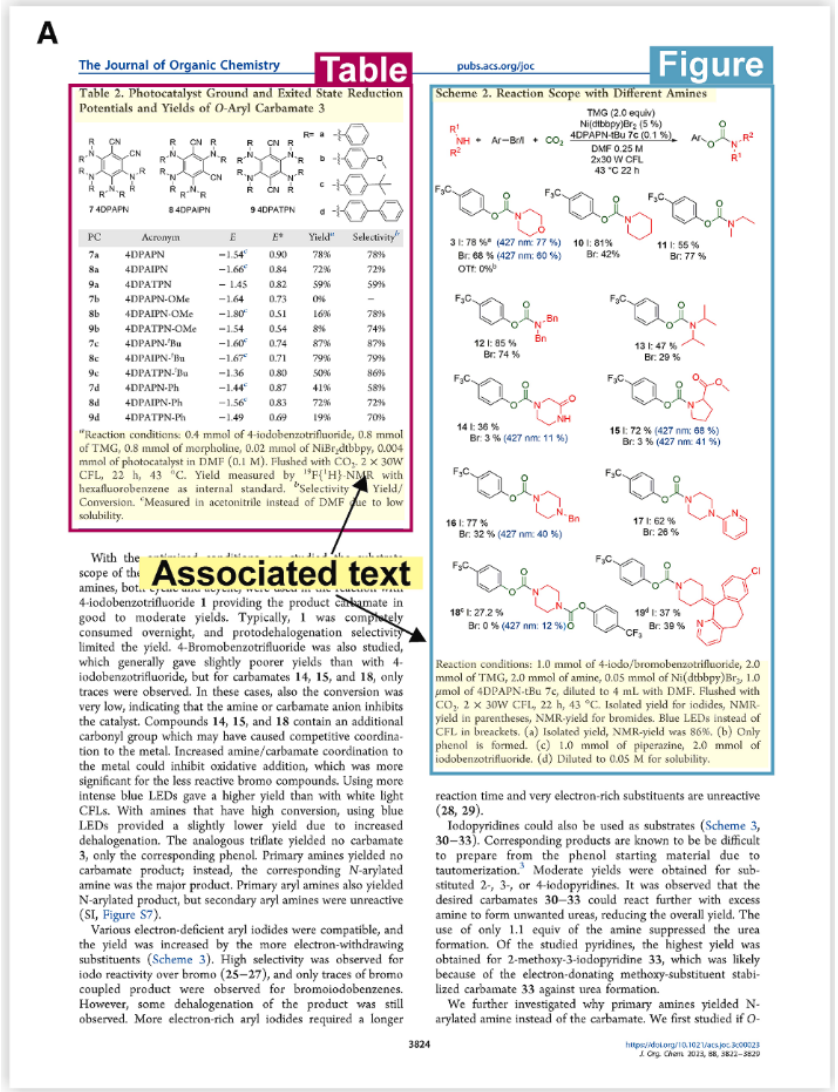
Keywords:
Electrochemical CO_2 reduction, Zenodo



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

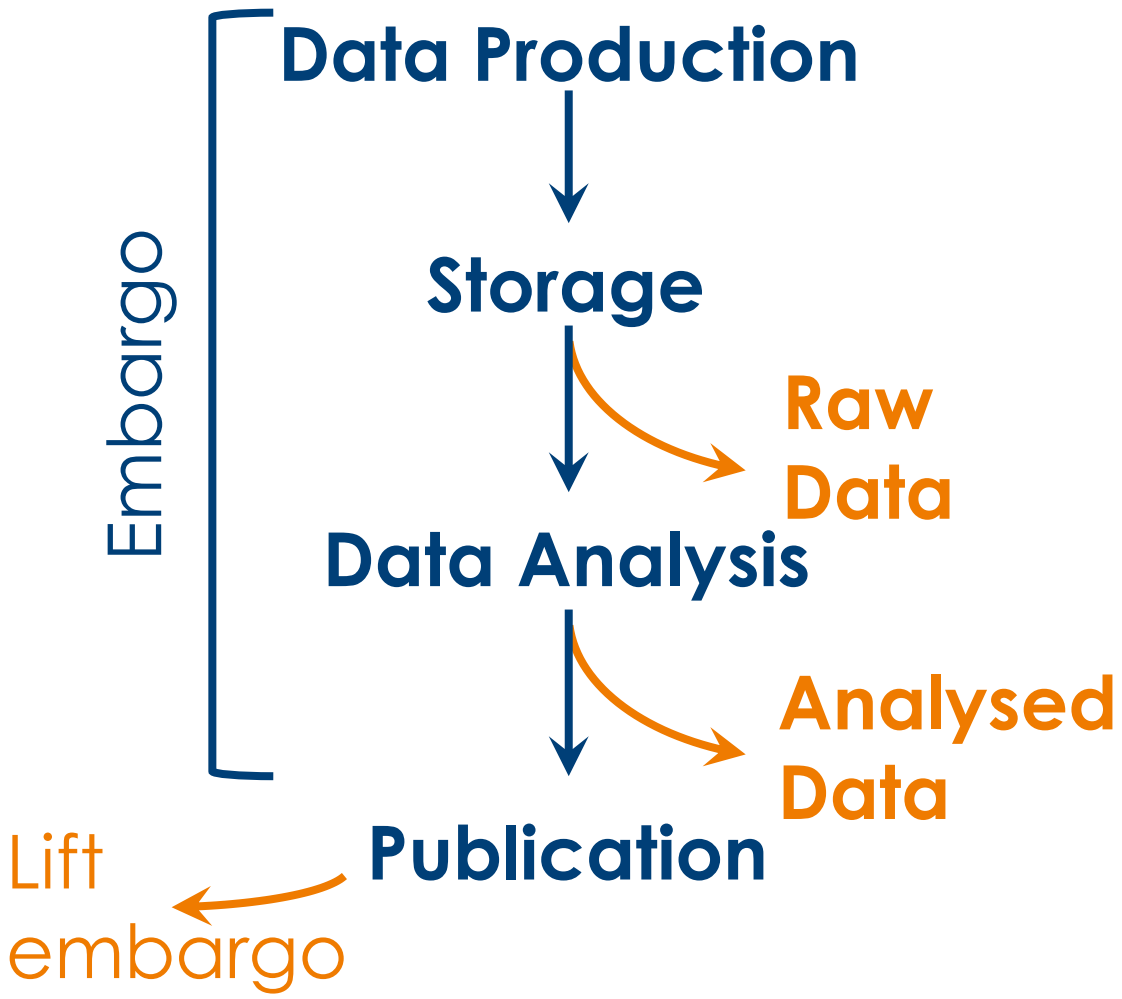
AI-based solution: MERMaid

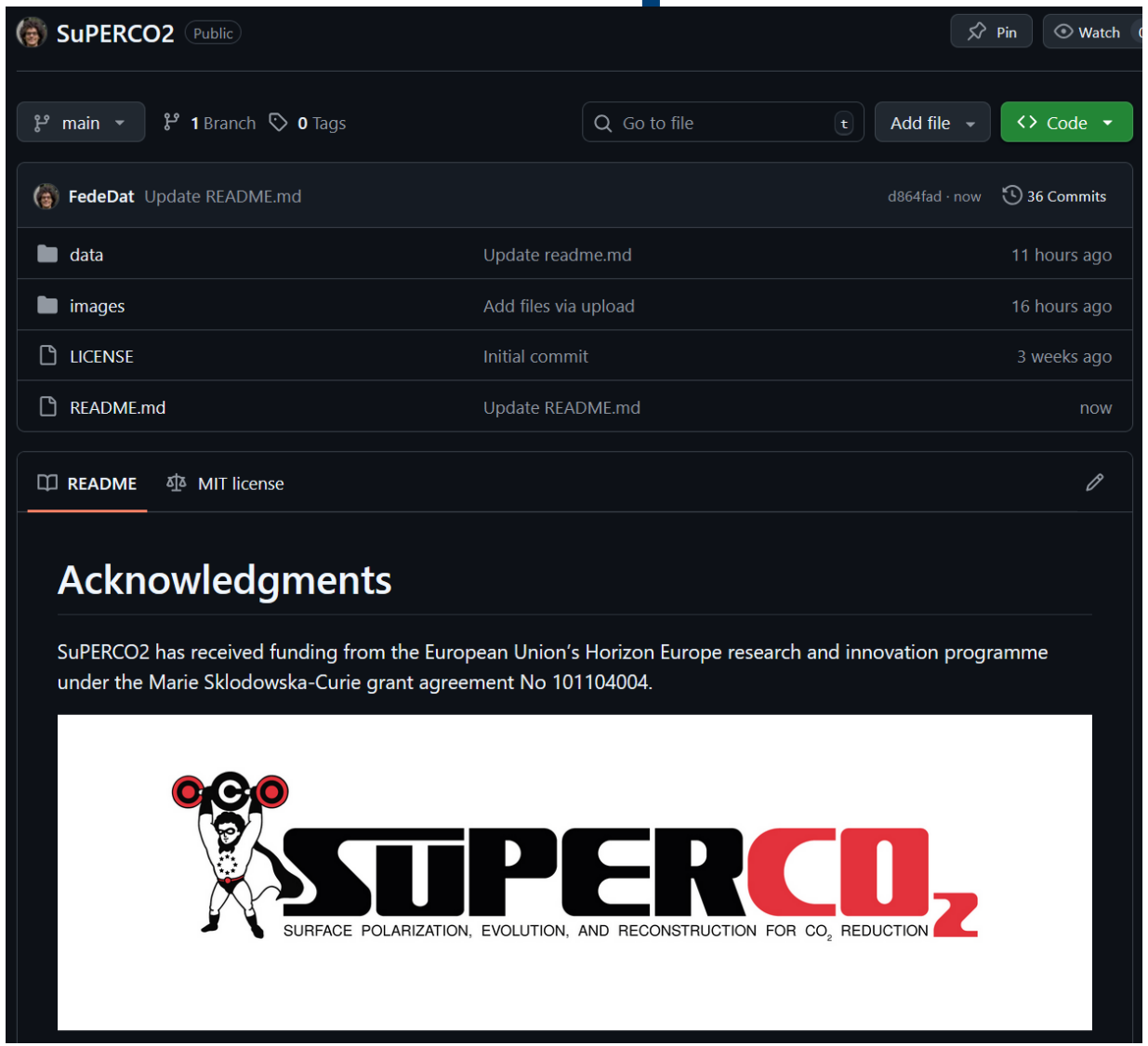




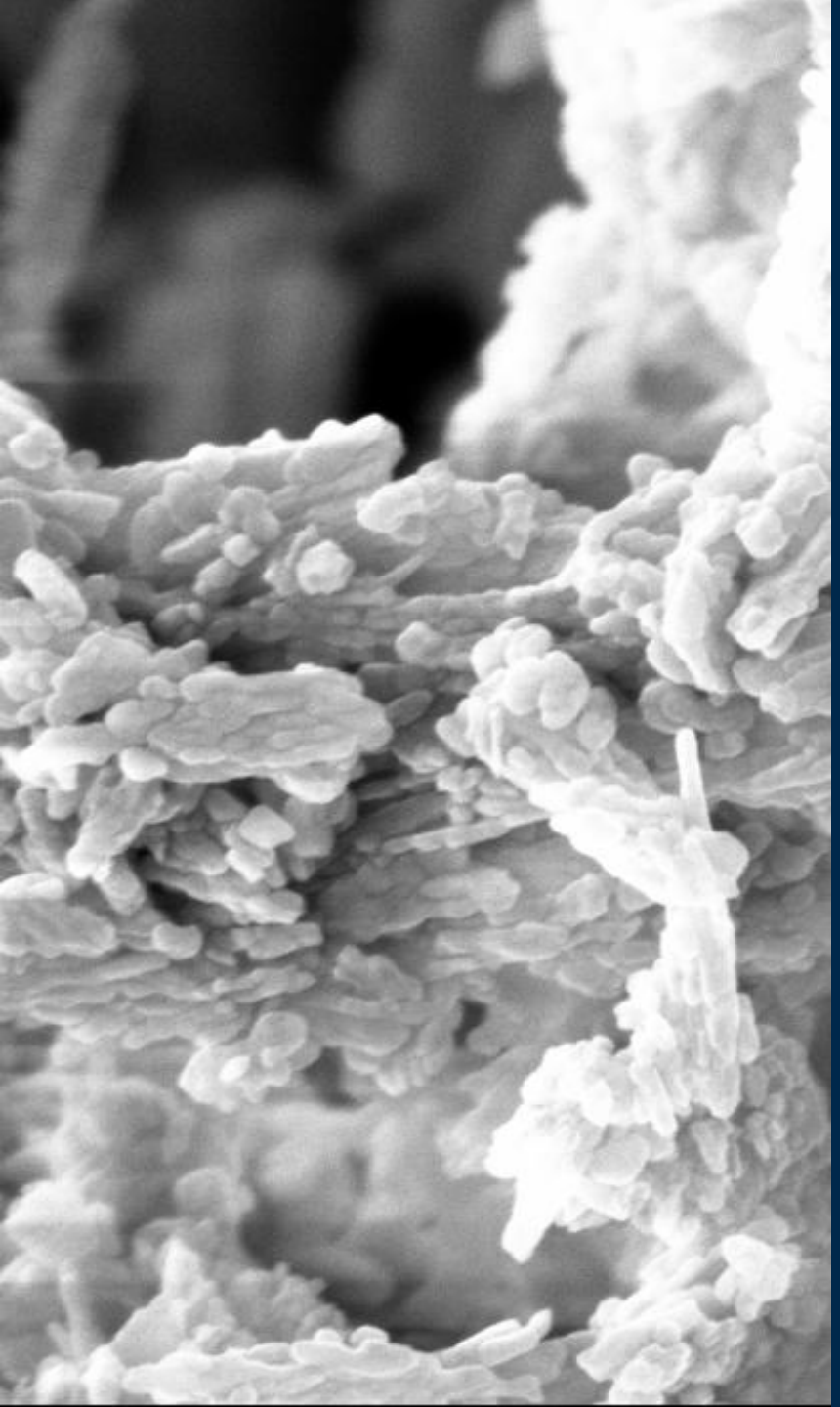
Leong, S. X.; Pablo-García, S.; Wong, B.; Aspuru-Guzik, A. *Matter* **2025**, *8*, 102331. https://doi.org/10.1016/j.matt.2025.102331.

The SuPERCO2 concept





SuPERCO2, https://github.com/FedeDat/SuPERCO2, online, accessed on 24/09/2025.



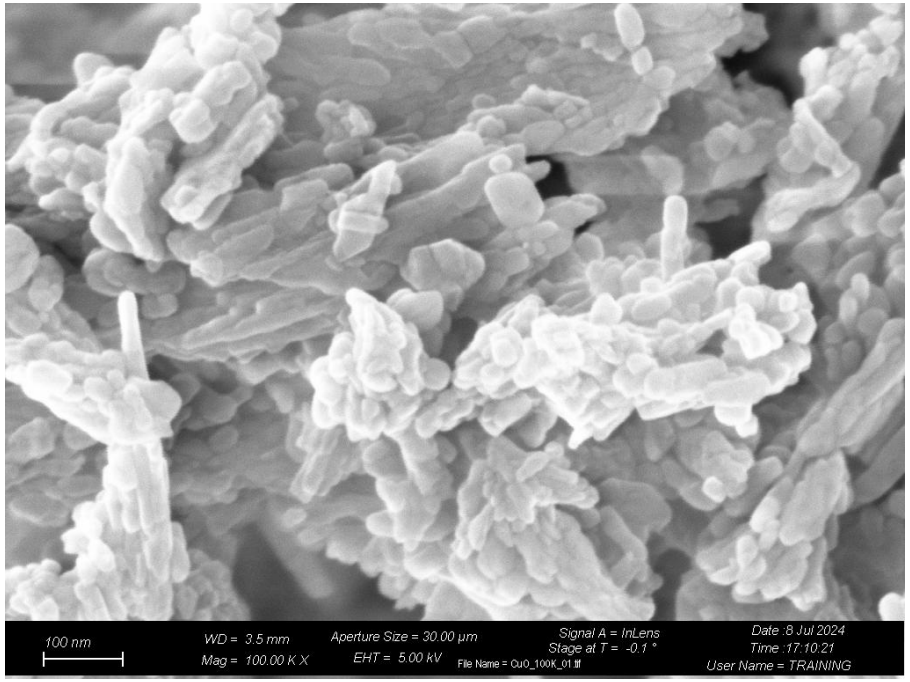
Characterization

Repository: github.com/FedeDat/SuPERCO2

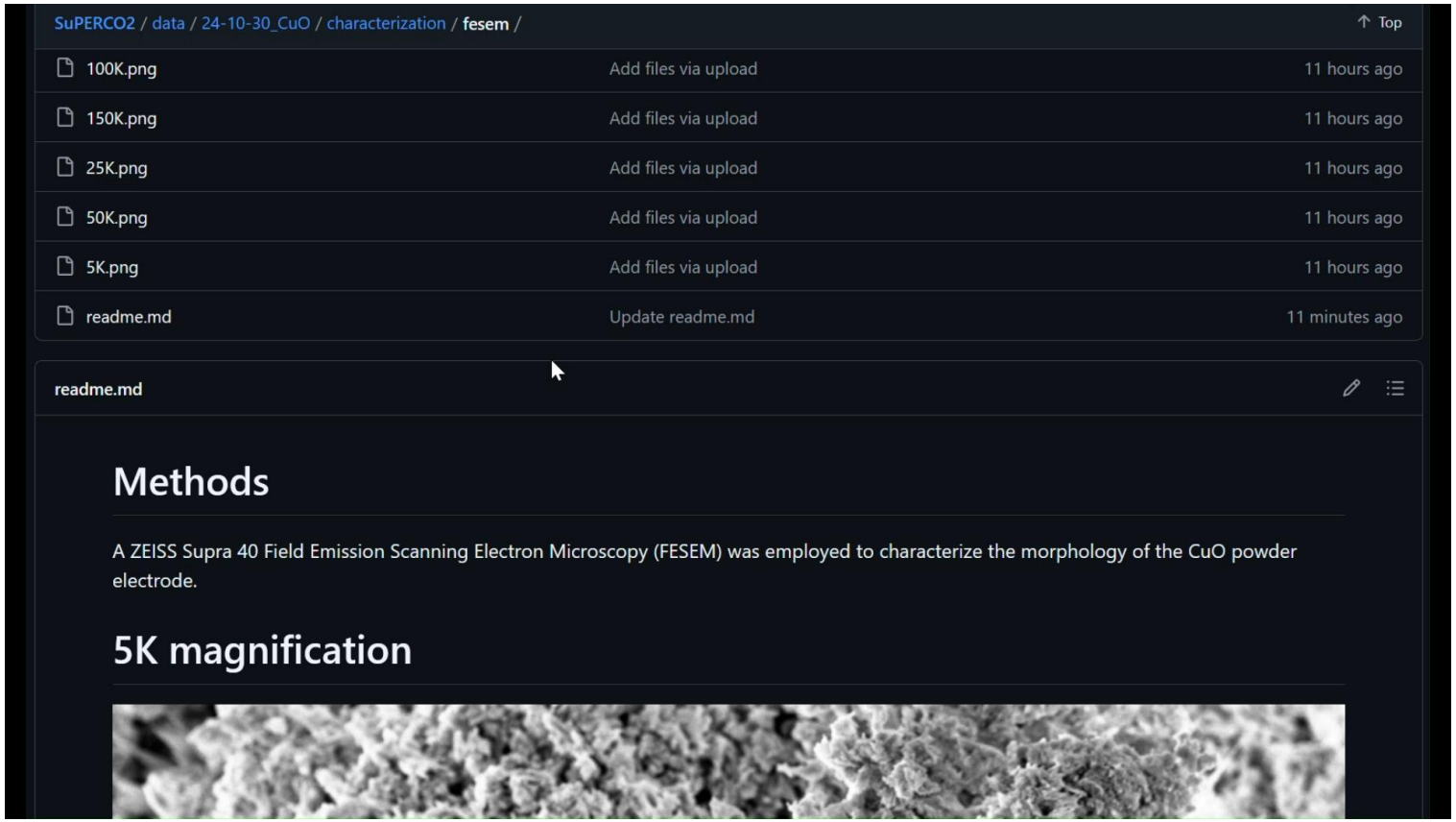
item: data/24-10-30_CuO/characterization

Scanning Electron Microscopy

Post-processing

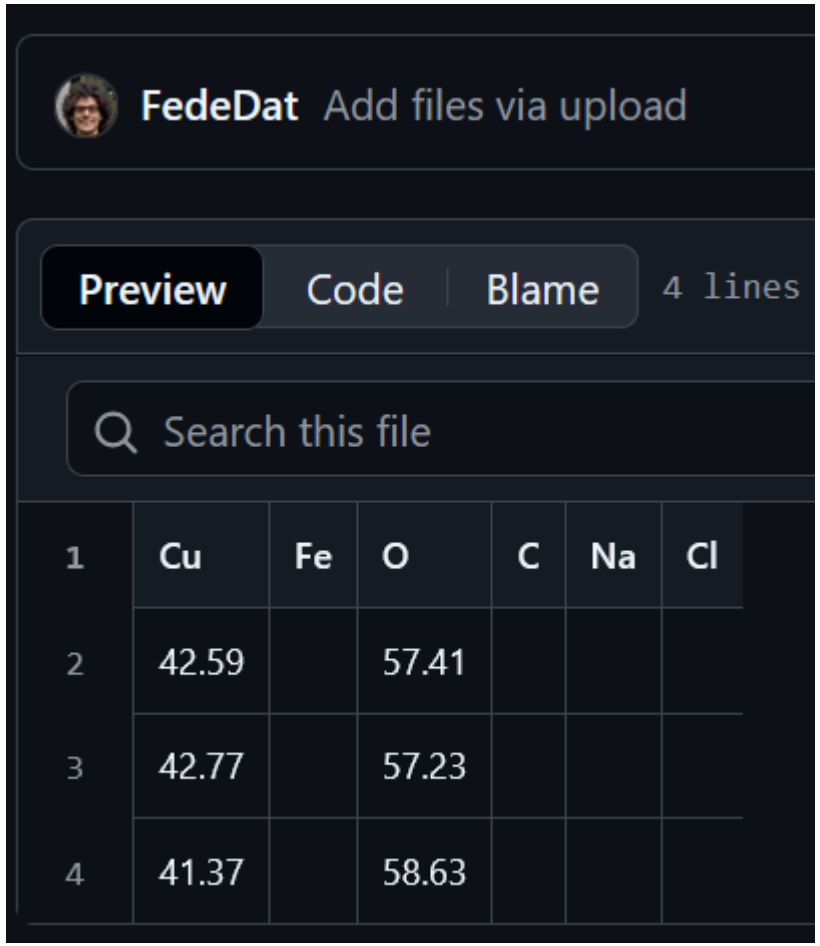


Data analysis & Visualization



Energy Dispersive X-ray

Post-processing



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.columns

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

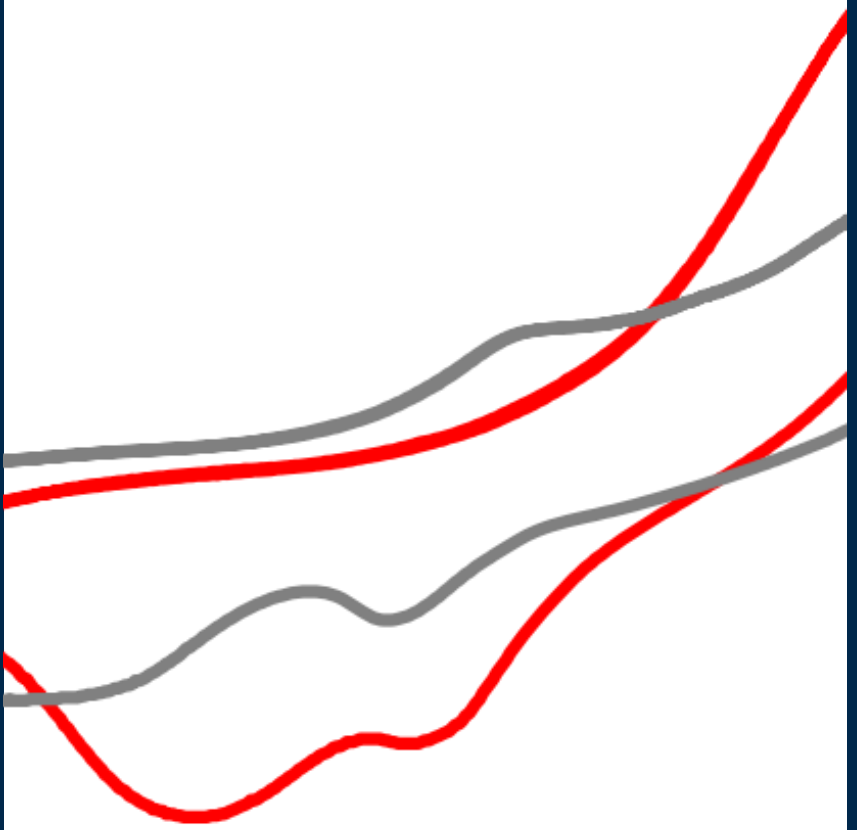
SuPERCO2 / data / 24-10-30_CuO / characterization / **XRD.csv**

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

	Angle	Intensity
29	20.01513028	862
30	20.04139085	848
31	20.06765141	881
32	20.09391198	856
33	20.12017254	853
34	20.14643311	891
35	20.17269367	876

Data analysis & Visualization

```python
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/24-10-30_CuO/EC

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

```
# 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()
```

https://github.com/FedeDat/SuPERCO2/data/24-10-30_CuO/EC

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

	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

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)))
```

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

Next steps

- Polish & upload Python scripts
- Provide a tutorial
- Automatize upload & analysis
- Create new modules: CP, etc.

Acknowledgements

Inspiration

M.Eng. Moisés Àlvarez (ICIQ)

Exp collaboration

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

Prof. Simelys Hernández
(lab Access)

Politecnico di Torino

DiSAT ECCELLENZA 2019 – 2027

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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)

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di Torino