

Organizational Information for CO₂ reduction Tafel slopes dataset

Aditya M. Limaye,[†] Joy S. Zeng,[†] Adam P. Willard,^{*,‡} and Karthish
Manthiram^{*,†}

[†]*Department of Chemical Engineering, MIT, Cambridge, MA*

[‡]*Department of Chemistry, MIT, Cambridge, MA*

E-mail: awillard@mit.edu; karthish@mit.edu

Dataset Organization

In this study, we manually digitized Tafel data included in several different papers from the electrochemical CO₂ reduction literature. Often, a single paper may report multiple sets of Tafel data, possibly with many traces in the same figure. Each distinct paper that reports (possibly multiple) Tafel data(set)s receives a unique three-digit identifier, which will be referred to as **PaperID**. Note that **PaperIDs** are *not* guaranteed to be consecutive, and some numbers are skipped. Within each paper, each dataset receives a separate three-digit identifier (unique within the same **PaperID**), which will be referred to as **SetID**. A single Tafel dataset in our study, then, is uniquely identified by the tuple (**PaperID**, **SetID**).

Our entire zipped dataset is organized into a hierarchical directory structure, with each directory named according to the **PaperID** identifier. Each individual paper directory contains several files. First, we include files with names of the form **figure*.png**, which are raw Portable Network Graphics (PNG) images of the paper figures, screenshotted manually from PDF copies of the papers. A few paper directories have multiple figure screenshots, and they are named according to **figure1.png**, **figure2.png**, etc. Directories also include raw data files with names of the form **dat_<SetID>.txt**, which contain raw x, y data taken from manually digitizing the figure. Associated with each raw data file is a separate metadata file with a name of the form **metadata_<SetID>.txt**. The metadata files contain key-value pairs stored in the YAML Ain't Markup Language (YAML) format, and contain several pieces of information required for processing the raw x, y data. YAML parsers are available in several programming languages, and the official YAML standard is documented at <https://yaml.org/>.

Metadata Tags

Tags in a metadata file are associated with YAML keys, and their associated values have several types. The types of the values, as well as the information they carry, are documented

in Table 1. Note that for CO₂ reduction catalysis, more negative applied electrochemical potentials correspond to more positive overpotentials. Studies in the literature report either the applied electrochemical potential or the overpotential on their voltage axis. The **v_reversed** tag contains the information required to properly orient the voltage data in the direction of increasing overpotential for each dataset.

Table 1: Table describing the types and meanings of the key-value pairs in the metadata files associated with each Tafel dataset.

Tag Name	Value Type	Value Meaning
<code>xdat</code>	Enum[‘current’, ‘voltage’]	Indicates which data is reported on the x axis.
<code>xunit</code>	String	String describing units of measurement for the x axis data, for example <code>mV</code> or <code>mA/cm2</code> .
<code>xlog</code>	Bool	Indicates whether the x axis data is reported on a logarithmic scale.
<code>ydat</code>	Enum[‘current’, ‘voltage’]	Indicates which data is reported on the y axis.
<code>yunit</code>	String	String describing units of measurement for the y axis data, for example <code>mV</code> or <code>mA/cm2</code> .
<code>ylog</code>	Bool	Indicates whether the y axis data is reported on a logarithmic scale.
<code>rval</code>	Float	Reported Tafel slope value.
<code>rerr</code>	Union[Float, None]	Error in reported Tafel slope value, if reported. If not reported, then <code>None</code> .
<code>runit</code>	String	String describing units of measurement for the x axis data, for example <code>mV/dec</code> .
<code>v_reversed</code>	Bool	If <code>false</code> , then the voltage data increases in value with increasing direction of the axis. If <code>true</code> , then the voltage data decreases in value with decreasing direction of the axis.
<code>i_reversed</code>	Bool	If <code>false</code> , then the current data increases in value with increasing direction of the axis. If <code>true</code> , then the current data decreases in value with decreasing direction of the axis.
<code>cat_tags</code>	List[String]	A list of tags describing the catalyst material. For example, a CuO catalyst would get the tags [‘Cu’, ‘O’].

Analyzed Papers

Table 2 documents the literature sources of all Tafel datasets analyzed in this study.

Table 2: Provenance of all Tafel datasets analyzed in this study. The PaperID defines the unique identifier assigned to the paper in the zipped dataset.

PaperID	Data Location	Document Object Identifier (DOI)
000	Figure 5	10.1021/ja5065284 ¹
002	Figure 4	10.1021/ja309317u ²
004	Figure 4	10.1246/bcsj.68.1889 ³
005	Figure 4	10.1002/anie.201604654 ⁴
009	Figure 5B	10.1021/acsnano.5b01079 ⁵
010	Figure 4B	10.1002/anie.201713003 ⁶
011	Figure 1C	10.1021/jacs.7b09074 ⁷
012	SI Figure 8	10.1002/anie.201900499 ⁸
014	Figure 10	10.1002/smll.201701809 ⁹
015	Figure 6D	10.1088/1361-6528/aa8f6f ¹⁰
016	Figure 7A	10.1021/jacs.5b02975 ¹¹
017	SI Figure 6	10.1002/smll.201602158 ¹²
021	Figure 5C	10.1002/celc.201700517 ¹³
022	Figure 3A, 3C	10.1002/cssc.201600202 ¹⁴
023	Figure 4A	10.1021/ja501923g ¹⁵
024	Figure 4B	10.1021/acsenerylett.8b00472 ¹⁶
025	SI Figure 12	10.1021/ja4113885 ¹⁷
026	Figure 2D	10.1016/j.elecom.2016.05.003 ¹⁸
027	Figure 3A, 3C	10.1021/ja2108799 ¹⁹
028	Figure 7A	10.1021/acs.jpcc.7b01586 ²⁰
029	SI Figure 13	10.1021/acscatal.7b00707 ²¹
031	Figure 7	10.1016/j.electacta.2016.03.182 ²²

032	Figure 8	10.1016/j.jcou.2017.05.024 ²³
033	Figure 2D	10.1002/cssc.201902859 ²⁴
035	Figure 4	10.1021/acsami.8b03461 ²⁵
036	SI Figure 8	10.1021/acsami.7b10421 ²⁶
039	Figure 3A	10.1002/asia.201800946 ²⁷
040	Figure 7	10.1002/cssc.201802409 ²⁸
042	SI Figure 4	10.1021/acsaem.8b00356 ²⁹
043	SI Figure 14	10.1021/acs.jpcc.8b06234 ³⁰
045	SI Figure 13	10.1021/acsaem.8b02048 ³¹
048	Figure 6C	10.1002/celc.201801132 ³²
049	Figure 4C	10.1002/adma.201706194 ³³
050	Figure 3	10.1038/ncomms4242 ³⁴
051	Figure 4	10.1021/acscatal.5b01235 ³⁵
052	Figure 4E	10.1002/aenm.201701456 ³⁶
053	Figure 3F	10.1016/j.chempr.2017.08.002 ³⁷
054	Figure 4C	10.1002/anie.201608279 ³⁸
055	Figure 7A	10.1016/j.apcatb.2018.01.001 ³⁹
056	Figure 4	10.1021/ja3010978 ⁴⁰
057	Figure 2C	10.1016/j.apcatb.2018.09.025 ⁴¹
058	Figure 5D	10.1021/jacs.6b10435 ⁴²
059	Figure 6	10.1021/jacs.6b12217 ⁴³
060	Figure 2F	10.1002/ange.201805696 ⁴⁴
061	Figure 6	10.20964/2017.03.72 ⁴⁵
062	Figure 3B	10.1002/cssc.201702229 ⁴⁶
063	Figure 3D	10.1002/aenm.201801536 ⁴⁷
064	Figure 4A	10.1016/j.jcis.2018.09.036 ⁴⁸
065	Figure 7	10.1016/j.nanoen.2018.03.023 ⁴⁹

066	Figure 3D	10.1021/jacs.7b12506 ⁵⁰
067	Figure 2D	10.1021/acscatal.5b00922 ⁵¹
068	Figure 3F	10.1021/acsnano.7b03029 ⁵²
069	Figure 4D	10.1021/acscatal.7b03449 ⁵³
070	Figure 8	10.1016/j.apsusc.2016.10.017 ⁵⁴
071	Figure 3	10.1002/anie.201802055 ⁵⁵
072	Figure 6A	10.1016/j.electacta.2018.04.047 ⁵⁶
074	Figure 2G	10.1021/jacs.5b08212 ⁵⁷
076	Figure 3A	10.1002/anie.201809255 ⁵⁸
077	Figure 4A	10.1002/anie.201711255 ⁵⁹
078	Figure 3G	10.1016/j.nanoen.2018.09.053 ⁶⁰
080	Figure 2H	10.1002/anie.201800367 ⁶¹
081	Figure 7	10.1016/j.cej.2016.02.084 ⁶²
083	Figure 2B	10.1016/j.apcatb.2017.06.032 ⁶³
084	Figure 2E	10.1016/j.jcat.2018.05.005 ⁶⁴
085	Figure 3E	10.1002/anie.201803873 ⁶⁵
086	Figure 3C	10.1002/anie.201806043 ⁶⁶
087	Figure 4D	10.1016/j.electacta.2018.09.080 ⁶⁷
088	Figure 5	10.1023/B:JACH.0000003866.85015.b6 ⁶⁸
089	Figure 6	10.1021/jp9822945 ⁶⁹
090	Figure 5C	10.1002/sml.201704049 ⁷⁰
091	Figure 5D	10.1016/j.nanoen.2016.11.004 ⁷¹
092	Figure 5B	10.1002/anie.201701104 ⁷²
093	Figure 3A	10.1021/jacs.6b12103 ⁷³
094	Figure 4A	10.1002/anie.201903613 ⁷⁴
095	SI Figure 8C	10.1002/anie.201900499 ⁸
096	Figure 2B	10.1002/adfm.201800499 ⁷⁵

097	SI Figure 6	10.1016/j.cattod.2015.05.017 ⁷⁶
098	Figure 4C	10.1021/acsami.7b16164 ⁷⁷
099	Figure 3	10.1002/sml1.201703314 ⁷⁸
100	Figure 4A	10.1016/j.apcatb.2018.08.075 ⁷⁹
101	Figure 4D	10.1073/pnas.1711493114 ⁸⁰
102	Figure 5B	10.1002/cssc.201800925 ⁸¹
103	Figure 1C	10.1021/acscatal.5b02424 ⁸²
104	Figure 3F	10.1021/acsenergylett.8b00519 ⁸³
105	Figure 4B	10.1002/anie.201612194 ⁸⁴
106	Figure 3C	10.1002/anie.201703720 ⁸⁵
108	SI Figure 4	10.1021/acs.nanolett.5b04123 ⁸⁶
109	Figure 3F	10.1002/anie.201901575 ⁸⁷
110	Figure 3D	10.1016/j.electacta.2018.12.116 ⁸⁸
111	Figure 5A	10.1021/acscatal.8b01022 ⁸⁹
112	Figure 3	10.1002/cssc.201701673 ⁹⁰
113	Figure 2D	10.1002/aenm.201900276 ⁹¹
114	Figure 2D	10.1021/acsenergylett.8b01286 ⁹²
115	Figure 2D	10.1002/anie.201712221 ⁹³
116	Figure 2D	10.1002/anie.201807571 ⁹⁴
117	Figure 3A	10.1021/acsenergylett.7b01096 ⁹⁵
118	Figure 5	10.1021/acsaem.8b01692 ⁹⁶
119	Figure 6	10.1039/C5CP03559G ⁹⁷
120	SI Figure 6	10.1126/science.aaw7515 ⁹⁸
121	Figure 10	10.1002/celc.201801036 ⁹⁹
122	Figure 5A	10.1002/adma.201705872 ¹⁰⁰
123	Figure 4C	10.1021/acscatal.8b04852 ¹⁰¹
124	Figure 2F	10.1016/j.jcou.2019.05.026 ¹⁰²

125	Figure 3D	10.1002/ange.201810538 ¹⁰³
126	Figure 3C	10.1016/j.joule.2018.11.008 ¹⁰⁴
127	Figure 1D	10.1002/aenm.201700759 ¹⁰⁵
128	Figure 5B	10.1002/celc.201700935 ¹⁰⁶
129	Figure 4B	10.1016/j.apcatb.2019.03.047 ¹⁰⁷
130	SI Figure 5B	10.1002/anie.201911995 ¹⁰⁸
131	SI Figure 12	10.1002/aenm.201702524 ¹⁰⁹
132	Figure 4C	10.1002/ange.201805256 ¹¹⁰
133	SI Figure 10	10.1002/aenm.201601103 ¹¹¹
134	Figure 2A	10.1038/s41467-018-07970-9 ¹¹²
135	Figure 2B	10.1016/j.nanoen.2019.05.003 ¹¹³
136	Figure 4	10.1039/C6TA04325A ¹¹⁴
137	Figure 2D	10.1002/celc.201800806 ¹¹⁵
138	Figure 3B	10.1002/anie.201805871 ¹¹⁶
139	Figure 4	10.1002/chem.201603359 ¹¹⁷
140	Figure 3D	10.1002/aenm.201903068 ¹¹⁸
141	Figure 3	10.1002/cssc.201501637 ¹¹⁹
142	Figure 3F	10.1002/anie.201907399 ¹²⁰
143	Figure 3E	10.1016/j.electacta.2018.08.002 ¹²¹
144	Figure 4A	10.1021/jp509967m ¹²²
145	SI Figure 8	10.1021/acs.est.5b00066 ¹²³
146	SI Figure 10	10.1021/acscatal.6b00543 ¹²⁴
147	SI Figure 39	10.1016/j.joule.2019.05.010 ¹²⁵
148	Figure 3B	10.1016/j.jcou.2019.02.007 ¹²⁶
149	Figure 4D	10.1002/cssc.201903117 ¹²⁷
150	Figure 3C	10.1002/chem.201803615 ¹²⁸
151	Figure 5D	10.1002/celc.201800104 ¹²⁹

152	Figure 4A	10.1039/C9EE00018F ¹³⁰
153	SI Figure 10	10.1016/j.joule.2018.10.015 ¹³¹
154	Figure 5	10.1002/celc.201900725 ¹³²
155	Figure 4B	10.1038/ncomms14503 ¹³³
156	Figure 2D	10.1016/j.elecom.2018.10.014 ¹³⁴
157	Figure 2C	10.1002/aenm.201803151 ¹³⁵
158	Figure 4E	10.1016/j.elecom.2019.03.017 ¹³⁶
159	Figure 4B, 4C	10.1002/cssc.201802725 ¹³⁷
160	Figure 12	10.1016/j.matchemphys.2017.02.016 ¹³⁸
161	Figure 4	10.1002/adfm.201802339 ¹³⁹
162	Figure 4D	10.1016/j.nanoen.2016.06.043 ¹⁴⁰
163	Figure 4C	10.1038/ncomms12697 ¹⁴¹
164	Figure 4F	10.1021/acssuschemeng.9b03502 ¹⁴²
165	Figure 5B	10.1039/C8TA03328E ¹⁴³
166	Figure 6C	10.1039/C7TA03005C ¹⁴⁴
167	Figure 3A	10.1002/anie.201908735 ¹⁴⁵
168	Figure 6D	10.1021/acsaem.9b02324 ¹⁴⁶
169	Figure 2C	10.1021/acs.jpcb.9b09730 ¹⁴⁷
170	Figure 3A	10.1073/pnas.1602984113 ¹⁴⁸
171	Figure 2	10.1021/acscatal.8b02181 ¹⁴⁹

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