Supporting Information:
Bayesian data analysis reveals no preference for cardinal Tafel slopes in CO\(_2\) reduction electrocatalysis

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1 Supplementary Discussion

2 Literature Analysis

3 Dataset Organization

In this study, we manually digitized Tafel data included in several different papers from the electrochemical CO\(_2\) 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(sets) 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 CO$_2$ 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.
Supplementary 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                                           |
|----------|------------------|---------------------------------------------------------|
| xdat     | Enum[‘current’, ‘voltage’] | Indicates which data is reported on the x axis.          |
| xunit    | String           | String describing units of measurement for the x axis data, for example mV or mA/cm². |
| xlog     | Bool             | Indicates whether the x axis data is reported on a logarithmic scale. |
| ydat     | Enum[‘current’, ‘voltage’] | Indicates which data is reported on the y axis.          |
| yunit    | String           | String describing units of measurement for the y axis data, for example mV or mA/cm². |
| ylog     | Bool             | Indicates whether the y axis data is reported on a logarithmic scale. |
| rval     | Float            | Reported Tafel slope value.                             |
| rerr     | Union[Float, None] | Error in reported Tafel slope value, if reported. If not reported, then None. |
| runit    | String           | String describing units of measurement for the x axis data, for example mV/dec. |
| v_reversed | Bool            | If false, then the voltage data increases in value with increasing direction of the axis. If true, then the voltage data decreases in value with decreasing direction of the axis. |
| i_reversed | Bool            | If false, then the current data increases in value with increasing direction of the axis. If true, then the current data decreases in value with decreasing direction of the axis. |
| cat_tags | List[String]     | A list of tags describing the catalyst material. For example, a CuO catalyst would get the tags [‘Cu’, ‘O’]. |
Table 2 documents the literature sources of all Tafel datasets analyzed in this study.

Supplementary 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<sup>1</sup>           |
| 002         | Figure 4          | 10.1021/ja309317u<sup>2</sup>            |
| 004         | Figure 4          | 10.1246/bcsj.68.1889<sup>3</sup>        |
| 005         | Figure 4          | 10.1002/anie.201604654<sup>4</sup>      |
| 009         | Figure 5B         | 10.1021/acsnano.5b01079<sup>5</sup>     |
| 010         | Figure 4B         | 10.1002/anie.201713003<sup>6</sup>      |
| 011         | Figure 1C         | 10.1021/jacs.7b09074<sup>7</sup>        |
| 012         | SI Figure 8       | 10.1002/anie.201900499<sup>8</sup>      |
| 014         | Figure 10         | 10.1002/smll.201701809<sup>9</sup>      |
| 015         | Figure 6D         | 10.1088/1361-6528/aa8f6f<sup>10</sup>   |
| 016         | Figure 7A         | 10.1021/jacs.5b02975<sup>11</sup>      |
| 017         | SI Figure 6       | 10.1002/smll.201602158<sup>12</sup>    |
| 021         | Figure 5C         | 10.1002/celc.201700517<sup>13</sup>    |
| 022         | Figure 3A, 3C     | 10.1002/cssc.201600202<sup>14</sup>    |
| 023         | Figure 4A         | 10.1021/ja501923g<sup>15</sup>        |
| 024         | Figure 4B         | 10.1021/acsenergylett.8b00472<sup>16</sup> |
| 025         | SI Figure 12      | 10.1021/ja4113885<sup>17</sup>         |
| 026         | Figure 2D         | 10.1016/j.elecom.2016.05.003<sup>18</sup> |
| 027         | Figure 3A, 3C     | 10.1021/ja2108799<sup>19</sup>        |
| 028         | Figure 7A         | 10.1021/acs.jpcc.7b01586<sup>20</sup>  |
| 029         | SI Figure 13      | 10.1021/acscatal.7b00707<sup>21</sup>  |
| 031         | Figure 7          | 10.1016/j.electacta.2016.03.182<sup>22</sup> |
| Page | Title       | DOI                        |
|------|-------------|----------------------------|
| 032  | Figure 8    | 10.1016/j.jcou.2017.05.024 |
| 033  | Figure 2D   | 10.1002/cssc.201902859    |
| 035  | Figure 4    | 10.1021/acsmi.8b03461     |
| 036  | SI Figure 8 | 10.1021/acsmi.7b10421     |
| 039  | Figure 3A   | 10.1002/asia.201800946    |
| 040  | Figure 7    | 10.1002/cssc.201802409   |
| 042  | SI Figure 4 | 10.1021/acsaem.8b00356   |
| 043  | SI Figure 14| 10.1021/acs.jpcc.8b06234 |
| 045  | SI Figure 13| 10.1021/acsaem.8b02048   |
| 048  | Figure 6C   | 10.1002/celc.201801132  |
| 049  | Figure 4C   | 10.1002/adma.201706194  |
| 050  | Figure 3    | 10.1038/ncomms4242       |
| 051  | Figure 4    | 10.1021/acscatal.5b01235 |
| 052  | Figure 4E   | 10.1002/aenm.201701456   |
| 053  | Figure 3F   | 10.1016/j.chempr.2017.08.002 |
| 054  | Figure 4C   | 10.1002/anie.201608279  |
| 055  | Figure 7A   | 10.1016/j.apcatb.2018.01.001 |
| 056  | Figure 4    | 10.1021/ja3010978        |
| 057  | Figure 2C   | 10.1016/j.apcatb.2018.09.025 |
| 058  | Figure 5D   | 10.1021/jacs.6b10435     |
| 059  | Figure 6    | 10.1021/jacs.6b12217     |
| 060  | Figure 2F   | 10.1002/ange.201805696   |
| 061  | Figure 6    | 10.20964/2017.03.72      |
| 062  | Figure 3B   | 10.1002/cssc.201702229   |
| 063  | Figure 3D   | 10.1002/aenm.201801536   |
| 064  | Figure 4A   | 10.1016/j.jcis.2018.09.036 |
| 065  | Figure 7    | 10.1016/j.nanoen.2018.03.023 |
|   | Figure/Reference | DOI                                |
|---|----------------|-----------------------------------|
|097 | SI Figure 6    | 10.1016/j.cattod.2015.05.017    |
|098 | Figure 4C      | 10.1021/acsami.7b16164           |
|099 | Figure 3       | 10.1002/sml1.201703314           |
|100 | Figure 4A      | 10.1016/j.apcatb.2018.08.075    |
|101 | Figure 4D      | 10.1073/pnas.1711493114          |
|102 | Figure 5B      | 10.1002/cssc.201800925           |
|103 | Figure 1C      | 10.1021/acscatal.5b02424         |
|104 | Figure 3F      | 10.1021/acsenergylett.8b00519    |
|105 | Figure 4B      | 10.1002/anie.201612194           |
|106 | Figure 3C      | 10.1002/anie.201703720           |
|108 | SI Figure 4    | 10.1021/acscatal.5b04123         |
|109 | Figure 3F      | 10.1002/anie.201901575           |
|110 | Figure 3D      | 10.1016/j.electacta.2018.12.116 |
|111 | Figure 5A      | 10.1021/acscatal.8b01022         |
|112 | Figure 3       | 10.1002/cssc.201701673           |
|113 | Figure 2D      | 10.1002/aenm.201900276           |
|114 | Figure 2D      | 10.1021/acsenergylett.8b01286    |
|115 | Figure 2D      | 10.1002/anie.201712221           |
|116 | Figure 2D      | 10.1002/anie.201807571           |
|117 | Figure 3A      | 10.1021/acsenergylett.7b01096    |
|118 | Figure 5       | 10.1021/acsam.8b01692            |
|119 | Figure 6       | 10.1039/C5CP03559G               |
|120 | SI Figure 6    | 10.1126/science.aaw7515          |
|121 | Figure 10      | 10.1002/celc.201801036           |
|122 | Figure 5A      | 10.1002/adma.201705872           |
|123 | Figure 4C      | 10.1021/acscatal.8b04852         |
|124 | Figure 2F      | 10.1016/j.jcou.2019.05.026      |
| Figure | Reference |
|--------|-----------|
| 3D     | 10.1002/ange.201810538 |
| 3C     | 10.1016/j.joule.2018.11.008 |
| 1D     | 10.1002/aenm.201700759 |
| 5B     | 10.1002/celc.201700935 |
| 4B     | 10.1016/j.apcatb.2019.03.047 |
| SI 5B  | 10.1002/anie.201911995 |
| SI 12  | 10.1002/aenm.201702524 |
| 4C     | 10.1002/ange.201805256 |
| SI 10  | 10.1002/aenm.201601103 |
| 2A     | 10.1038/s41467-018-07970-9 |
| 2B     | 10.1016/j.nanoen.2019.05.003 |
| 4      | 10.1039/C6TA04325A |
| 2D     | 10.1002/celc.201800806 |
| 3B     | 10.1002/anie.201805871 |
| 4      | 10.1002/chem.201603359 |
| 3D     | 10.1002/aenm.201903068 |
| 3      | 10.1002/cssc.201501637 |
| 3F     | 10.1002/anie.201907399 |
| 3E     | 10.1016/j.electacta.2018.08.002 |
| 4A     | 10.1021/jp509967m |
| SI 8   | 10.1021/acs.est.5b00066 |
| SI 10  | 10.1021/acscatal.6b00543 |
| SI 39  | 10.1016/j.joule.2019.05.010 |
| 3B     | 10.1016/j.jcou.2019.02.007 |
| 4D     | 10.1002/cssc.201903117 |
| 3C     | 10.1002/chem.201803615 |
| 5D     | 10.1002/celc.201800104 |
| 152 | Figure 4A | 10.1039/C9EE00018F<sup>130</sup> |
| 153 | SI Figure 10 | 10.1016/j.joule.2018.10.015<sup>131</sup> |
| 154 | Figure 5 | 10.1002/celc.201900725<sup>132</sup> |
| 155 | Figure 4B | 10.1038/ncomms14503<sup>133</sup> |
| 156 | Figure 2D | 10.1016/j.elecom.2018.10.014<sup>134</sup> |
| 157 | Figure 2C | 10.1002/aenm.201803151<sup>135</sup> |
| 158 | Figure 4E | 10.1016/j.elecom.2019.03.017<sup>136</sup> |
| 159 | Figure 4B, 4C | 10.1002/cssc.201802725<sup>137</sup> |
| 160 | Figure 12 | 10.1016/j.matchemphys.2017.02.016<sup>138</sup> |
| 161 | Figure 4 | 10.1002/adfm.201802339<sup>139</sup> |
| 162 | Figure 4D | 10.1016/j.nanoen.2016.06.043<sup>140</sup> |
| 163 | Figure 4C | 10.1038/ncomms12697<sup>141</sup> |
| 164 | Figure 4F | 10.1021/acssuschemeng.9b03502<sup>142</sup> |
| 165 | Figure 5B | 10.1039/C8TA03328E<sup>143</sup> |
| 166 | Figure 6C | 10.1039/C7TA03005C<sup>144</sup> |
| 167 | Figure 3A | 10.1002/anie.201908735<sup>145</sup> |
| 168 | Figure 6D | 10.1021/acsaem.9b02324<sup>146</sup> |
| 169 | Figure 2C | 10.1021/acs.jpcb.9b09730<sup>147</sup> |
| 170 | Figure 3A | 10.1073/pnas.1602984113<sup>148</sup> |
| 171 | Figure 2 | 10.1021/acscatal.8b02181<sup>149</sup> |

**Data Licensing**

Code that supports the findings of this study is available under the MIT License in Zenodo (http://doi.org/10.5281/zenodo.3995021). Data that supports the findings of this study is available under CC BY 4.0 (https://creativecommons.org/licenses/by/4.0/) in Zenodo (http://doi.org/10.5281/zenodo.3995021), with the exception of the excerpted figures from other articles as described in the Supporting Information. The excerpted fig-
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**Residuals vs. Literature-Reported Values**

Residual analysis can help sniff out systematic or correlated errors in the results presented in Fig. 3A of the main text. We can define residuals between the literature-reported values and the MAP values in several different ways. Here, we will consider two definitions of the residuals, normalized either to the literature-reported Tafel slopes,

$$\text{Residual Normalized to Reported} = \frac{T_{\text{reported}} - T_{\text{MAP}}}{T_{\text{reported}}},$$  \hspace{1cm} (1)

or to the MAP Tafel slopes,

$$\text{Residual Normalized to MAP} = \frac{T_{\text{reported}} - T_{\text{MAP}}}{T_{\text{MAP}}}. \hspace{1cm} (2)$$

Figure 1 depicts plots of the residuals versus the literature-reported and MAP Tafel slopes (A and C, respectively), as well as kernel density estimates of the distribution over the residuals normalized to the literature-reported and MAP Tafel slopes (B and D, respectively). To the eye, the residuals appear roughly unbiased around zero, and there appear to be no spurious correlations between the residuals.

**Correlation Plot over Full Range**

Figure 2 depicts a correlation plot of the MAP Tafel slope versus the literature-reported Tafel slope, including all datasets considered in this study.
Supplementary Figure 1: Residual Analysis. (A) Plot of the relative residual to the literature-reported Tafel slope, defined in Eq. (1), versus the literature-reported Tafel slope, including only reported Tafel slopes less than 200 mV/decade. (B) Kernel density estimate of the distribution over the relative residual to the literature-reported Tafel slope. (C) Plot of the relative residual to the MAP Tafel slope, defined in Eq. (1), versus the MAP Tafel slope, including only reported Tafel slopes less than 200 mV/decade. (D) Kernel density estimate of the distribution over the relative residual to the MAP Tafel slope.
Supplementary Figure 2: Correlation plot of reported Tafel slopes from the literature against Tafel slopes fitted by our algorithm on identical data. The solid red line represents perfect agreement, while the red filled intervals are lines representing 10% and 20% relative error.
For every single dataset considered in the study, we draw $N = 4 \times 10^4$ samples from the posterior distribution over the Tafel slope. In Fig. 3C in the main text, we depict a kernel density estimate of the distribution over the MAP Tafel slope from each of these posterior distributions. We choose to display this data because the MAP Tafel slope is a straightforward point estimate of the Tafel slope given a posterior distribution over the parameter, and hence is likely the quantity one would quote if asked what the Tafel slope of a catalyst is. However, the averaging operation involved in computing the MAP Tafel slope can collapse broad features in the posterior distribution down to a single value; this is especially true in the case of bimodal posterior distributions arising from insufficient datasets. Figure 3 depicts a kernel density estimate of the distribution over the Tafel slope using all samples collected from the posterior distribution for each dataset. The essential conclusions reported in the main text are upheld when examining the data in Fig. 3. A very small preference for Tafel slopes around 45 mV/decade emerges in this analysis. However, given the small amount of total distributional mass under this peak and the high degree of sampling variability (as evinced by the bootstrap standard deviations), we do not believe it should be interpreted strongly.

**Catalyst Breakout Results**

As described in the main text, we split out our results on the distributions over the Tafel slope by catalyst material identity in order to confirm that our conclusion of a lack of Tafel cardinality in CO$_2$ reduction catalysis is not an artifact of pooling together data from several catalyst materials, each of which individually exhibit cardinality. Figures 4–9 depict these results for catalysts containing Cu, Ag, Au, Sn, and Bi. Each figure has three panels: the left-most panel plots a kernel density estimate of the distribution over Tafel slopes using all samples from the posterior distribution, akin to Fig. 3. The center panel plots a kernel density estimate of the distribution over the MAP Tafel slope from each dataset, akin to main
Supplementary Figure 3: Kernel density estimates (KDE) of the empirical probability distribution function of Tafel slopes reported in literature data (blue) and those refitted by our algorithm (red). Error intervals correspond to one standard deviation of bootstrapped resamples. Green dashed lines correspond to cardinal values of the Tafel slope.
text Fig. 3C. The right-most panel plots a CDF of the distributional breadth $B_i$ for each dataset considered. The distributional breadth is parametrized by the threshold parameter $t$, and is defined as,

$$B_i(t) = \text{CDF}_i^{-1}(1 - t) - \text{CDF}_i^{-1}(t),$$

where $\text{CDF}_i(m_T)$ represents the CDF of the Tafel slope for the $i$'th dataset. Intuitively, a high distributional breadth implies that the experimental data measured in the dataset does not provide information to pin down the value of the Tafel slope with high confidence. Correspondingly, if the CDF of the distributional breadth increases quickly, then most of the datasets in the catalyst material subset predict tight distributions over the Tafel slope. Conversely, if the CDF of the distributional breadth climbs slowly, then several datasets in the catalyst material subset do not determine a Tafel slope value with high confidence.

For some catalysts, the KDE constructed from all Tafel slope samples (left panel) and the KDE constructed from the MAP Tafel slope samples (center panel) show different behavior. The former plot looks more visually noisy than the latter plot; this is to be expected, since taking the mean of the posterior distribution over the parameters is a “smoothing” operation. The two ways of visualizing the data convey slightly distinct information, since the KDE constructed from all samples preserves the uncertainty information retained in a single fit, while the KDE constructed from the MAP Tafel slopes is the most direct comparison to the distribution of literature values (which do not carry an associated uncertainty, in most cases). In certain cases (Ag, Sn), the KDE comprising all samples appears to have more defined peaks than the KDE comprising MAP samples. First, we note that in these cases, the bootstrap standard errors for these peaks are much greater than in other areas of the distribution, suggesting that this peaking behavior is controlled by a small number of samples, and hence more variable with respect to a change in the specific datasets re-analyzed in this study. Second, peaking behavior in the KDE comprising all samples that does not appear in the KDE comprising MAP samples is a sign of some underlying data insufficiency issues highlighted by Fig. 2 in the main text; these peaks can easily disappear.
or be shifted upon measuring additional data. To declare confidently that a certain dataset espouses a cardinal Tafel slope preference, we contend that both ways of visualizing the distribution of Tafel slopes for a certain catalyst should show peaking around a cardinal value. This standard, while stringent, enforces that the available experimental data confidently determines a cardinal value of the Tafel slope, free of latent data insufficiency issues. While we observe this for the Bi breakout results in Fig. 9, the remainder of the catalyst breakout datasets do not meet this standard. Hence, though we do not foreclose the possibility that additional future data collection on these catalysts may reveal a cardinal Tafel slope preference, we argue that broadly, when considering the data extant in the literature, the typical CO₂ reduction catalyst does not exhibit a strong preference for cardinal values of the Tafel slope.

Supplementary Figure 4: Tafel Slope statistics for catalysts containing Ag ($N_{\text{datasets}} = 38$). (Left) Kernel density estimates (KDE) of the empirical probability distribution function of Tafel slopes reported in literature data (blue) and those refitted by our algorithm (red). Error intervals correspond to one standard deviation of bootstrapped resamples. Green dashed lines correspond to cardinal values of the Tafel slope. (Center) Same as (Left), but KDEs are computed using only the MAP Tafel Slope values for each dataset. (Right) CDF of the distributional breadth, as defined by Eq. (3).
Supplementary Figure 5: Tafel Slope statistics for catalysts containing Au ($N_{\text{datasets}} = 50$). (Left) Kernel density estimates (KDE) of the empirical probability distribution function of Tafel slopes reported in literature data (blue) and those refitted by our algorithm (red). Error intervals correspond to one standard deviation of bootstrapped resamples. Green dashed lines correspond to cardinal values of the Tafel slope. (Center) Same as (Left), but KDEs are computed using only the MAP Tafel Slope values for each dataset. (Right) CDF of the distributional breadth, as defined by Eq. (3).

Supplementary Figure 6: Tafel Slope statistics for catalysts containing Ag or Au ($N_{\text{datasets}} = 88$). (Left) Kernel density estimates (KDE) of the empirical probability distribution function of Tafel slopes reported in literature data (blue) and those refitted by our algorithm (red). Error intervals correspond to one standard deviation of bootstrapped resamples. Green dashed lines correspond to cardinal values of the Tafel slope. (Center) Same as (Left), but KDEs are computed using only the MAP Tafel Slope values for each dataset. (Right) CDF of the distributional breadth, as defined by Eq. (3).
Supplementary Figure 7: Tafel Slope statistics for catalysts containing Cu ($N_{\text{datasets}} = 54$). (Left) Kernel density estimates (KDE) of the empirical probability distribution function of Tafel slopes reported in literature data (blue) and those refitted by our algorithm (red). Error intervals correspond to one standard deviation of bootstrapped resamples. Green dashed lines correspond to cardinal values of the Tafel slope. (Center) Same as (Left), but KDEs are computed using only the MAP Tafel Slope values for each dataset. (Right) CDF of the distributional breadth, as defined by Eq. (3).

Supplementary Figure 8: Tafel Slope statistics for catalysts containing Sn ($N_{\text{datasets}} = 37$). (Left) Kernel density estimates (KDE) of the empirical probability distribution function of Tafel slopes reported in literature data (blue) and those refitted by our algorithm (red). Error intervals correspond to one standard deviation of bootstrapped resamples. Green dashed lines correspond to cardinal values of the Tafel slope. (Center) Same as (Left), but KDEs are computed using only the MAP Tafel Slope values for each dataset. (Right) CDF of the distributional breadth, as defined by Eq. (3).
Supplementary Figure 9: Tafel Slope statistics for catalysts containing Bi ($N_{\text{datasets}} = 27$). (Left) Kernel density estimates (KDE) of the empirical probability distribution function of Tafel slopes reported in literature data (blue) and those refitted by our algorithm (red). Error intervals correspond to one standard deviation of bootstrapped resamples. Green dashed lines correspond to cardinal values of the Tafel slope. (Center) Same as (Left), but KDEs are computed using only the MAP Tafel Slope values for each dataset. (Right) CDF of the distributional breadth, as defined by Eq. (3).
**Limiting Current Statistics**

Figure 10 depicts kernel density estimates of the distribution of fitted limiting currents $i_{\text{lim}}$ from a re-analysis of literature data. Roughly, the distribution appears to be in agreement with the value of the transport-limited current density for CO$_2$ reduction at an aqueous flooded electrode.

Supplementary Figure 10: Limiting current statistics for all datasets analyzed in the study. (Left) Kernel density estimates (KDE) of the empirical probability distribution of the limiting current, $i_{\text{lim}}$ fitted when interpreting the data through the model in main text Eq. (2). (Right) Same as (Left), but KDEs are computed using only the MAP limiting current values for each dataset.

**Bayesian Fitting**

**Mathematical Detail**

As quoted in the main text, Bayes’ rule reads,

$$p(\theta|y) = \frac{p(y|\theta) \times p(\theta)}{p(y)}.$$  \hspace{1cm} (4)

In the context of this work, $y$ represents the measured current data at a set of voltage points. We will use the subscript notation $y_k$ to denote a single current data point, where the index $k = 1, \ldots, N_{\text{pts}}$. The parameters of a model for interpreting current-voltage data are denoted
by $\theta$; in the context of this work, the relevant parameters for the limiting current model are $i_{\text{lim}}$, the limiting current density, $i_0$, the exchange current density, and $m^{-1}_T$, the inverse Tafel slope. We will denote the model’s predictions at each voltage point by the subscript notation $M_k(\theta)$.

To successfully apply Bayes’ rule to glean $p(\theta|y)$, the posterior distribution over the model parameters given measured data, we need to identify mathematical forms for the prior distribution $p(\theta)$ and the likelihood function $p(y|\theta)$. In all fits conducted in this study, we employ a uniform prior distribution (also known as an “uninformative” prior distribution) over a certain parameter range. Since the prior is uniform in the selected parameter range, as long as the range includes the values of the parameters for which $p(\theta|y)$ has high probability mass, the choice of prior is unimportant (see further on for a numerical confirmation of this fact). Given this fact, the choice for the range of our uniform prior is determined by first using a standard nonlinear least-squares optimization algorithm (TRF) to determine a point estimate of the optimal set of parameters, $\theta^*$. Formally,

$$\theta^* = \arg\min_{\theta} \left\{ \sum_{k=1}^{N_{\text{pts}}} [y_k - M_k(\theta)]^2 \right\}.$$  \hspace{1cm} (5)

With the optimal parameters $\theta^*$ in hand, we select a uniform prior $p(\theta)$ that is supported in the range $[0, a \times \theta^*_i]$ for each parameter $i = 1, \ldots, N_{\text{params}}$. We choose the very conservative value $a = 10$ to ensure that the prior distribution has support over a very broad range around the optimal parameters. In principle, this choice of $a$ results in a wide parameter space, which may affect the computational efficiency of a posterior sampling algorithm. In practice, we find very little computational disadvantage for choosing $a = 10$ as compared to $a = 2$ when using the No-U-Turn Sampler implemented in PyMC3.

The likelihood function for the data given the parameters, $p(y|\theta)$, is determined by assuming that the experimental measurement represents a ground truth measurement described
by the model, polluted by unavoidable experimental error,

\[ y_k = M_k(\theta) + \epsilon_k. \]  

(6)

We assume that errors at different data points are uncorrelated, and further assume that the error \( \epsilon_i \) at any single data point is drawn from a Gaussian distribution with zero mean and variance \( \sigma^2 \),

\[ p(\epsilon_k) = \frac{1}{\sqrt{2\pi}\sigma} \exp \left[ -\frac{\epsilon_k^2}{2\sigma^2} \right]. \]  

(7)

Because the errors at each point are uncorrelated, the likelihood now factorizes over all the data points,

\[ p(y|\theta) = \prod_{k=1}^{N_{\text{pts}}} \frac{1}{\sqrt{2\pi}\sigma} \exp \left[ -\frac{(y_k - M_k(\theta))^2}{2\sigma^2} \right]. \]  

(8)

With a likelihood function \( p(y|\theta) \) and a prior distribution \( p(\theta) \) in hand, we can plug this information into a Monte Carlo sampler of our choice to draw samples from the posterior distribution \( p(\theta|y) \). Equation (8) also makes apparent how one can generalize the Bayesian posterior sampling approach to more general models \( M(\theta) \). After we write down a suitable model, we simply evaluate the model predictions with different parameters whenever we need to compute the likelihood function for a given set of parameters during the sampling procedure.

**Gaussian Error Estimates from Nonlinear Optimization**

The Bayesian posterior sampling approach advanced in this work provides a way to glean distributional uncertainty information about the estimated values of model parameters given observed data. A similar set of information can also be obtained by analyzing the Hessian matrix determined by a nonlinear optimization algorithm seeking an optimal point estimate.
of the model parameters. Specifically, if the optimizer seeks to minimize a loss function,

\[ \mathcal{L}(\theta) = \frac{1}{2\sigma^2} \sum_{k=1}^{N_{\text{pts}}} [y_k - \mathcal{M}_k(\theta)]^2 , \]  

(9)

then it often also produces an estimate of the Hessian,

\[ H_{ij} = \left. \frac{\partial \mathcal{L}}{\partial \theta_i \partial \theta_j} \right|_{\theta^*} , \]  

(10)

evaluated at the optimal value of the parameters \( \theta^* \). If we assume that the experimental data is generated by the random process described by Eq. (6), and further assume that the errors at different data points are uncorrelated and drawn from Gaussian distributions with mean zero and variance \( \sigma^2 \), then we can form a Gaussian approximation to the posterior distribution around \( \theta^* \),

\[ p(\theta|y) \approx \frac{1}{(2\pi)^{d/2}(\det H)^{1/2}} \exp \left[ -\frac{1}{2} (\theta - \theta^*)^T H (\theta - \theta^*) \right] , \]  

(11)

where \( d \) is the number of parameters being estimated, and \( H \) is guaranteed to be positive definite by virtue of being evaluated at the optimal point \( \theta^* \).

We stress that the expression provided by Eq. (11) is an approximation to the true posterior distribution; due to its Gaussian form, this expression can never accurately represent bimodality in the posterior distribution. In this sense, the Bayesian sampling approach is superior, although it comes at significant additional computational expense as \( d \) increases. In this work, \( d = 3 \), and this additional expense is essentially negligible given the computational power available on a typical laptop or desktop computer. Hence, we suggest that posterior distributions over the Tafel slope fitted using the model in Eq. (2) of the main text should always be computed using the Bayesian posterior sampling algorithm described in the previous section. We have simply included mention of the Gaussian approximation for the sake of completeness, and to guide possible future work that attempts to fit models
Sensitivity to Error Distribution Width

One important parameter of the Bayesian fitting approach is the width of the normal distribution governing the probability of deviations from the model, which arises when evaluating the quantity $p(y|\theta)$ in Bayes’ rule. Figure 11 studies the sensitivity of the posterior distribution over the Tafel slope to the parameter $\sigma$, the standard deviation of the normal distribution governing the statistics of the model error. As expected, lowering the value of $\sigma$ causes the algorithm to become more confident in its estimate. At $\sigma = 0.01$ logarithmic units, the model essentially nails the true Tafel slope of 80 mV/decade. For larger values of $\sigma$, a clear distributional drift to lower values of the Tafel slope is observed. This occurs because most of the data in Fig. 11A lies in the plateau region, and the model faces less penalty for down-weighting these points as the value of $\sigma$ is increasing. Hence, the model drifts to larger slopes on the Fig. 11A plot, which corresponds to lower values of the Tafel slope. Note that the distributional widening is significantly greater than the drift in the mean, suggesting that we should not put much stock into the mean drift. The upshot: for high values of the...
σ parameter, this particular set of data does not contain enough information to pin down the value of the Tafel slope accurately.

**Sensitivity to Prior Distribution**

As explained in the main text, our Bayesian approach requires specification of a prior distribution $p(\theta)$ over the parameters. Since we know very little about the true distribution of the Tafel slope at the outset, we choose an uninformative uniform box prior over the interval $[0, a \times \theta^*_i]$ for each parameter $\theta_i$, where $\theta^*_i$ is the optimal value of the parameter gleaned from the TRF algorithm described in the Methods section. Here, we conduct a sensitivity analysis on the $a$ parameter. Given that we are using an uninformative prior, we should expect that the prior width should not influence the posterior distribution as long as the data expresses some opinion about the ideal value of the parameters. Figure 12 depicts the results of the sensitivity analysis on a set of synthetic data. Indeed, as expected, the posterior distributions are insensitive to the choice of prior. Note that in all fits considered in the main text, we use a value of $a = 10$, as mentioned in the Methods section.

Supplementary Figure 12: Sensitivity to the width of the uniform prior distribution bounds. (A) Synthetic data sampled from a model with an underlying Tafel slope of 80 mV/decade. (B) Several traces of the posterior distribution computed using different values of $a$, a parameter influencing the width of the prior distribution fed to the Bayesian posterior sampling algorithm. All posterior distributions are computed with $\sigma = 0.05$. 
Derivations

Cardinal Tafel Slopes Equation

We will work with a generic reaction scheme, assuming that we begin with a starting species $A^{(n+q)+}$ which undergoes $n$ electron transfers prior to the rate-determining step, and then $q$ electron transfers at the RDS. In practice $n$ will be an integer, and $q$ will be either zero or one. Here we assume the reaction taking place is reductive; however, the derivation is entirely analogous for an equivalent oxidation reaction. Schematically, the reactions read,

$$
A^{(n+q)+} + e^- \leftrightarrow A^{(n+q-1)+} \\
\vdots \\
A^{(q+1)+} + e^- \leftrightarrow A^q \\
A^q + q e^- \rightarrow A.
$$

The overall current is determined by the rate of the RDS. Assuming Butler-Volmer kinetics for the forward rate constant of the RDS, we have,

$$
\text{rate} = k_0 \left\{ a_{A^q+} \exp \left[-\beta q e (1 - \alpha) \cdot (\phi - \phi_{eq})\right] - a_A \exp \left[+\beta q e \alpha \cdot (\phi - \phi_{eq})\right] \right\},
$$

where $k_0$ is the rate prefactor (sometimes called the Arrhenius prefactor), $a_i$ is the activity of species $i$, $\beta \equiv (k_B T)^{-1}$ is the inverse thermodynamic temperature, $e$ is the fundamental charge, $\alpha$ is the symmetry coefficient, $\phi$ is the applied potential, and $\phi_{eq}$ is the equilibrium potential for the RDS. At sufficiently high reductive overpotentials $\phi - \phi_{eq} \ll 0$, only the first term survives,

$$
\text{rate} \approx k_0 a_{A^q+} \exp \left[-\beta q e (1 - \alpha) \cdot (\phi - \phi_{eq})\right].
$$

To make further progress, we have to solve for the activity of the intermediate species $A^{q+}$ in terms of the activity of the reactant species for the overall reaction, $A^{(n+q)+}$. If we assume
that all steps prior to the RDS are fast and equilibrated, we can extract this activity by analyzing the thermodynamics of the steps prior to the RDS. The free energy change associated with the $r$’th reaction reads,

$$\Delta F_r = -\beta^{-1} \log a_{A^{(n+q-(r+1)+}}} + \beta^{-1} \log a_{A^{(n-q-r)+}} + e\phi. \quad (14)$$

Then, the equilibrium constant for reaction $r$ goes as,

$$K_r \equiv \exp [-\beta \Delta F_r] \quad (15)$$

$$K_r = \frac{a_{A^{(n+q-(r+1)+}}}{a_{A^{(n-q-r)+}}} \times \exp [-\beta e\phi] \quad (16)$$

$$K_r = \tilde{K}_r \times \exp [-\beta e\phi], \quad (17)$$

where $\tilde{K}_r$ is defined by Eq. (17), and is independent of potential. Since Eq. (17) holds for all reactions $r$ before the RDS, we can easily solve for the activity of the intermediate,

$$a_{A^{q+}} = \left[ \prod_{r=1}^{n} \tilde{K}_r \right] \exp [-n\beta e\phi] \times a_{A^{(n+q)+}} \quad (18)$$

$$a_{A^{q+}} = \left[ \prod_{r=1}^{n} \tilde{K}_r \right] \exp [-n\beta e(\phi - \phi_{eq.})] \exp [-n\beta e\phi_{eq.}] \times a_{A^{(n+q)+}}. \quad (19)$$

Plugging back into Eq. (13),

$$rate \approx k_0 \left( \prod_{r=1}^{n} \tilde{K}_r \right) \exp [-n\beta e(\phi - \phi_{eq.})] \exp [-n\beta e\phi_{eq.}] \times a_{A^{(n+q)+}} \exp [-\beta qe(1 - \alpha) \cdot (\phi - \phi_{eq.})]$$

$$rate = k_0 \left( \prod_{r=1}^{n} \tilde{K}_r \right) \exp [-n\beta e\phi_{eq.}] \times a_{A^{(n+q)+}} \exp [-\beta e(\phi - \phi_{eq.})(n + q \cdot (1 - \alpha))]. \quad (21)$$

This is a mess, but we only care about the potential-dependent terms when extracting the Tafel slope, which means we only have to consider the last factor on the RHS. Taking the
logarithm yields,

$$\log [\text{rate}] = -\beta e (\phi - \phi_{eq}) (n + q \cdot (1 - \alpha)) + C,$$

where $C$ is a constant independent of potential. For a reduction reaction, the Tafel slope is defined as,

$$\text{Tafel Slope} = \left( \frac{\partial \log_{10} [\text{rate}]}{\partial \left( - (\phi - \phi_{eq}) \right)} \right)^{-1}.$$

Hence, we have,

$$\text{Tafel Slope} = \left[ \log_{10} (\exp(1)) \cdot \beta e \right]^{-1} \cdot \frac{1}{n + q \cdot (1 - \alpha)}.$$

Appropriate unit scalings yield,

$$\text{Tafel Slope} = \frac{60 \text{ mV/decade}}{n + q \cdot (1 - \alpha)},$$

which reduces to the equation quoted in the main text when $\alpha = 1/2$.

**Physical Non-Idealities**

**Tafel Slopes with Physical Non-Idealities**

Eq. (25) already accounts for the non-ideality effects introduced by $\alpha \neq 1/2$. If we assume that the CO$_2$ adsorption step has partial charge transfer character quantified by $\gamma$, then despite the fact that the adsorption step is purely chemical, we assume that its equilibrium constant carries a non-integer order dependence on the applied potential. This can also be motivated by considering the formation of a permanent dipole on the surface species, which can access additional thermodynamic stabilization due to a dipole Stark shift from electric fields present at the interface. The manner in which surface dipole formation augments the Tafel slope depends on whether or not the CO$_2$ adsorption step is the rate determining step. For the case $(n, q) = (0, 1)$, the adsorption step is the RDS. The Frumkin correction
attenuates the applied potential for the rate-determining step by a factor \( f \), which simply multiplies the latter term in the denominator of Eq. (25). Hence, the Tafel slope for \((n, q) = (0, 1)\) is,

\[
\text{Tafel Slope} = \frac{60 \text{ mV/decade}}{\gamma \cdot f \cdot (1-\alpha)}. \tag{26}
\]

For the case \((n, q) = (1, 0)\), the adsorption step is the RDS, and rather than contributing \( n = 1 \) to the order, it instead contributes according to the \( \gamma \) parameter,

\[
\text{Tafel Slope} = \frac{60 \text{ mV/decade}}{\gamma}. \tag{27}
\]

Finally, for the case \((n, q) = (1, 1)\), the adsorption step occurs before the RDS, and the Tafel slope reads,

\[
\text{Tafel Slope} = \frac{60 \text{ mV/decade}}{\gamma + f \cdot (1-\alpha)}. \tag{28}
\]

Sensitivities to Parameter Bounds

Figures 13 and 14 study the sensitivity of the distributional results presented in Fig. 4 of the main text to the bounds of the uniform distributions over non-ideality parameters. Broadly, our claim is supported by the sensitivity analysis; within reasonable parameter bounds, we still see that we can get essentially arbitrary distributional shapes depending on the nonidealities included in the model.

Multiple Kinetic Regimes

Here, we examine the consequences of fitting current-voltage data from a system exhibiting multiple kinetic regimes to a model that only allows a single Tafel slope (as in Eq. (2) in the main text) by analyzing synthetic data. The synthetic data is generated from the model,

\[
\frac{1}{i(E)} = \frac{1}{i_{\text{lim}}} + \frac{1 + \exp \left( -e \frac{k_B T}{1} \times |E - E_{\text{eq,1}}| \right)}{\exp \left( e \frac{k_B T}{1} \times \alpha |E - E_{\text{eq,2}}| \right)}, \tag{29}
\]
Supplementary Figure 13: Several synthetic kernel density estimates of the probability distributions over the Tafel slope generated from including random values of different parameters governing physical non-idealities. Different panels use different uniform distributions over the symmetry coefficient parameter, $\alpha$.

Supplementary Figure 14: Several synthetic kernel density estimates of the probability distributions over the Tafel slope generated from including random values of different parameters governing physical non-idealities. Different panels use different uniform distributions over the Frumkin correction parameter, $f$. 
where $E$ is the applied potential, and the model has free fitting parameters $\alpha$, $i_{\text{lim}}$, $E_{\text{eq},1}$, and $E_{\text{eq},2}$. This model can be shown to arise when a reaction proceeds through a rate-limiting surface reaction involving a surface intermediate generated through a one-electron transfer, and present at non-negligible surface coverages. The specifics of how this model arises are less relevant to this analysis than the fact that the model exhibits two different Tafel regimes. When $\alpha = 1/2$, the first regime has Tafel slope $m_T = 40 \text{ mV decade}^{-1}$ for $E_{\text{eq},1} < E < E_{\text{eq},2}$, and the second regime has a Tafel slope $m_T = 120 \text{ mV decade}^{-1}$ for $E > E_{\text{eq},2}$, before topping out at the limiting current $i_{\text{lim}}$.

**Supplementary Figure 15:** (A) Current-voltage trace generated from Eq. (29) using the parameters $\alpha = 1/2$, $i_{\text{lim}} = 100 \text{ mA cm}^{-2}$, $E_{\text{eq},1} = 0.05 \text{ V}$, and $E_{\text{eq},2} = 0.15 \text{ V}$ (red trace), along with artificially noised data sampled from the model (black points). (B) Current-voltage traces evaluated from the MAP fit parameters for Eq. (2) in the main text and Eq. (29), along with the noised data used for the fits (black points). (C) Posterior distribution over the Tafel slope for the model described by Eq. (2) in the main text.

Figure 15A shows a trace of the current-voltage behavior predicted by Eq. (29), with parameters $\alpha = 1/2$, $i_{\text{lim}} = 100 \text{ mA cm}^{-2}$, $E_{\text{eq},1} = 0.05 \text{ V}$, and $E_{\text{eq},2} = 0.15 \text{ V}$, as well as artificially noised data sampled from this model at a sparsely sampled set of voltage points. Figure 15B shows current-voltage traces from both Eq. (29) (red) and Eq. (2) from the main text (blue), each evaluated under the MAP parameters determined from their respective Bayesian fits. Finally, Fig. 15C shows the Bayes posterior distribution for the Tafel slope fitted using Eq. (2) from the main text. As expected, when using the single Tafel regime model to fit data generated from multiple Tafel regimes, the MAP value of the Tafel slope does not coincide with the Tafel slope from either kinetic regime in Eq. (29).
Supplementary Figure 16: Posterior distributions for $\alpha$, $i_{\text{lim}}$, $E_{\text{eq},1}$, and $E_{\text{eq},2}$ (A, B, C, D, respectively) gleaned from Bayesian posterior sampling on the artificially noised data in Fig. 15A.
However, as illustrated in Fig. 16, when the original data is fit to Eq. (29), the posterior distributions are peaked around the true values of the parameters.

This analysis yields two important takeaways. First, it lends credence to the idea that fitting a single Tafel slope to data collected under multiple Tafel regimes, each individually exhibiting a cardinal Tafel slope, can produce an off-cardinal value of the Tafel slope, providing an alternative possible explanation for the lack of observed cardinality in the literature analysis in the main text. Second, and perhaps more importantly, it shows that the Bayesian framework presented here can successfully estimate the parameters of more complicated physical models that incorporate the effects of multiple different Tafel regimes, or some of the physical nonidealities discussed in the main text. Practically, we furnish the following recommendation: if one knows in advance that multiple kinetic regimes are at play in a set of current-voltage data, and the nature of these regimes can be encoded into a kinetic model like Eq. (29), then one should carry out Bayesian fitting to such a model. In the absence of sufficient independent evidence to pin down a kinetic model that resolves multiple kinetic regimes, Eq. (2) from the main text is a viable alternative, but one should be very cautious about over-interpreting the mechanistic implications of a Tafel slope determined in this manner.
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