

Week 6

Intro to Long Reports

6.1 Lecture 10: Scientific Visual Communication

2/7:

- Long report submissions delayed until Friday.
 - The content of today may be useful!
- Thursday.
 - Anna Wuttig on the current state of EChem.
 - Tokmakoff will stick around after for us to chat about our reports with him.
- There are many aspects beyond *visual* communication, but this is one that isn't always seen, so Tokmakoff decided to focus on it today.
- Take all the guidelines and extra chapters seriously; they're exactly what is being graded for.
- We should care about communication because it's as important to our career development as anything.
 - Our science must be distributed; otherwise, we're just a hobbyist.
- We need to convey very complicated, quantitative information to other scientists, management, government agencies, policy makers, investors, and the general public.
- Reduce complex quantitative data accurately into clear, concise messages: Data interpretation.
- Often, there are real requirements on content and formatting.
- Excellence in communication.
 - Content is key, but saying it well will really level you up.
 - It develops *trust* in your methods, results, and communications.
 - A well-communicated report and graphic can change the world, e.g., the hockey stick curve.
- **Communication:** The means of exchanging information.
- **Medium:** Any channel of communication.
- Media we will discuss.
 - Print (text, graphics).
 - Graphics are how people digest scientific information.
 - Oral (in person with visual support).
 - Never use double columns if you want transport to online.

- The common starting point for all communication.
 1. Audience.
 - Identify; sets the objective, expectations, language, and aspects of your work to focus on.
 - You need to know if you're talking to fellow bench scientists, or senior management.
 2. Message.
 - What are you trying to say? Just say what you need to, and get rid of the rest.
 - When your TA or Tokmakoff reads your report, what are they going to think of my magenta line.
 3. Media.
 - What tools are at your disposal, and how are they best employed.
- Visual presentation tips for text and graphics.
 - Our goal: Communicate quantitative information clearly and concisely.
 - Make your viewer's life easy (be consistent, define the purpose of each element, etc.).
 - Simplicity is good; clutter is bad.
 - Color should be chosen with a real focus in mind.
- Typefaces and fonts.
 - The visual representation of language. Its style should help, not interfere, with your communication.
- **Typeface**: The design elements for lettering. A collection of glyphs.
- **Glyph**: A single representation of a character.
- **Font**: A variation of a typeface like size, weight, and spacing.
- Classes of typefaces: **Serif** and **sans serif**.
 - Sans-serif is good for titles, headings, and labels.
 - Serifs are good for presenting large amounts of text.
- History of typefaces.
 - Use legacy typefaces; they're still supported.
 - "Microsoft is your friend."
 - Computers revolutionized typography; Microsoft drove the development with proprietary stuff, which eventually caused them to lose the edge, and now there's great open-source fonts.
- Typefaces for equations.
 - Times New Roman and Garamond have full math support.
 - Computer modern (\TeX) is probably still the best in terms of being able to distinguish things since it includes so many helpful flourishes.
 - You're probably encountered difficulties with the lab manual (e.g., v vs. ν) because it's not in Computer modern.
- Tokmakoff's recommendations for formatting: Typed 8.5×11 documents should have a...
 - Single column format.
 - 1" margins.
 - 11-12 point type.

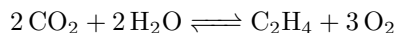
- ~ 90 characters per line including spaces (15 characters per linear inch).
 - 4-5 lines per vertical inch.
- Why worry about font size?
 - Legibility vs. readability; too small impacts legibility, and too big impacts readability.
- Why worry about line spacing?
 - $1.5\times$ is Tokmakoff's recommendation.
 - $2\times$ is legacy from typewriters, when single and double were the only options.
- Why worry about margins?
 - White space helps with clarity.
 - Don't just insert figures; make figures break text.
- Equations should be numbered.
- Color.
 - Don't let it distract; let it help you make a cleaner presentation.
 - Really bright colors draw the eye too much.
- Scientific figures.
 - Purpose: To convey quantitative information on the relationship between different physical variables with minimal effort.
 - Each figure should convey information on exactly one topic.
 - Again, know your audience, be aware of your medium (typed vs. oral), clarity, etc.
 - Additional consideration for scientific reports: Often the figure is the only documentation of the data.
 - If the reader wanted to analyze your data, can they read data values off the graph using the axis labels?
 - Raw Excel sheets, other records may not be saved, so the literature report may be the only way for future scientists to reanalyze your data.
- Examples of good and bad figures.
 - As you see scientific figures going forward, take note of what you like and what you don't like and learn.
 - Tokmakoff asks for the class's feedback on his examples.
- You should have 4-6 axis labels and 4-10 tick marks.
 - More tick marks than labels is a good idea!
- Make sure colors translate to black and white, so maybe I should vary both shapes and colors in my Birge-Sponer plot.
- Rowan is very picky about what Excel settings you use.
 - Don't cut and paste into word; stuff gets realigned.
- Tokmakoff doesn't look for units for unitless quantities (e.g., absorbance).
- Use a legend when there are two or more series being plotted.
- Caption.

- Use for report figures.
- It should describe what is plotted and is needed to interpret the data beyond what is in the figure.
- For data, typically quote specific experimental conditions.
- Titles are only for oral presentation graphics.
- Don't mislead! Rescaling your axes can mislead about growth.
- Make everything 300 dpi.
- Publishers use JPG in CMYK color profile.
 - Online: Use RGB color profile.
 - Everything else is up to us.
- Takeaways.
 - Clarity and conciseness.
 - White space is good!
 - Microsoft is (mostly) your friend.
 - Their templates, colors, and fonts have been professionally designed... with everyone in mind.
 - Use recommended formatting, but be aware it isn't for scientists.
 - There are no firm rules — just guidelines. It is an art.

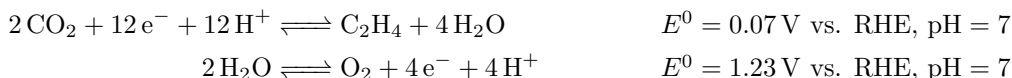
6.2 Lecture 11: Electrochemistry

2/9:

- Guest lecture by Anna Wuttig.
- Ben Masters (our TA) is one of her grad students.
- Electrochem can solve important problems, and we know the mechanisms in principle because we can measure the flow of electrons in it as current.
 - Thus, we can modify whatever we want and have an *in situ* handle on reaction rate.
 - This is why it's important for physical chemistry, which seeks to understand, predict, and rationally design future reactions.
- We will focus on CO₂-reduction today.
 - Wuttig hopes to **upconvert** it to other things.
- We currently do this with the water-gas shift reaction and Fischer-Tropsch chemistry.
 - But this is both energy-intensive and has poor selectivity.
- Alternative: Electrochemistry.
- Example.

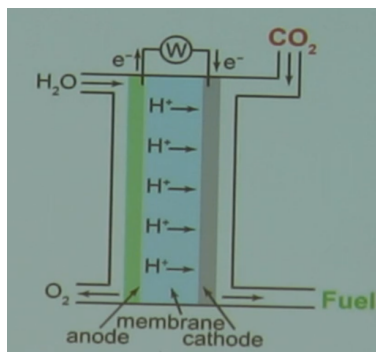


- Produces ethylene (used in a lot of things in industry) and O₂ (benign).
- Allows you to store $\Delta G = 1343 \text{ kJ mol}^{-1}$ of energy, corresponding to $\Delta E = -1.16 \text{ V}$.
- This involves two electrochemical half-reactions (recall from gen-chem).



- The first one is kinetically very difficult, though — it requires you to input *twelve* electrons.

- In the EChem module, we'll study RHEs and other kinds of electrodes.
 - Essentially, these allow us to pin EChem reactions on a common axis.
 - The axis does move as a function of pH, though.
- We have no electrolyser or catalyst that can run the example reaction right now.
 - Thus, we so far have to put in more energy to store that energy.
 - A focus of the chemistry world: Find catalysts and conditions such that this is possible.
- CO₂ reduction as an energy storage scheme.

Figure 6.1: CO₂ reduction as an energy storage scheme.

- Use renewable energy sources like wind and solar to drive electrochemical reactions. Specifically, driving the transfer of electrons may facilitate oxidation of water to O₂ at the anode reduction of CO₂ to fuels (such as ethylene) at the cathode. Note that the water's protons will theoretically diffuse through a proton exchange membrane.
- Big idea: Store renewable intermittent electricity in energy-dense chemical bonds.
- Selectivity challenges in CO₂ reduction.
 - One reason we don't know how to do this yet: CO₂ can be reduced to myriad products.
 - A competitive side reaction: Hydrogen evolution.
 - Other carbonaceous products include methanol, ethanol, etc. Some of these may be good, but we don't want to produce all of them at once!
 - Though it might be theoretically possible to pin the ΔE thermodynamically, it's practically virtually impossible.
 - Consequently, selective CO₂RR requires control over the relative rates (kinetics) of competing reactions.
- Understanding of interfacial proton coupling is poor.
 - $\text{CO}_2 + 2\text{e}^- + 2\text{H}^+ \longrightarrow \text{CO} + \text{H}_2\text{O}$ is possible.
 - Things like molecular electrocatalysts allow us to access this at a high rate and selectivity.
 - We can boost the rate even further with *intramolecular* proton donors (esp. phenolic groups).
 - *Intermolecular* proton donors can help, too, but make sure not to make it too acidic, or you'll favor hydrogen evolution!
 - Thus, what you really need is precise proton delivery.
 - These homogeneous catalysts are nice and pretty, but in a functional device, we'll need heterogeneous catalysis.

- Possible example: Au catalyst.
 - Mathematical models suggest that the concentration profiles at the interface of the solid are higher. Essentially, the pH near the surface becomes much more alkaline very quickly
 - We don't have control over the proton coordinate here, and we don't actually know what the proton donor is (could be water, hydronium, carbonic acid, etc.).
 - Thus, we need to understand the role of PCET in dictating CO₂RR vs. HER selectivity.
 - This is what Wuttig did her PhD on!
- Electrochemistry is nice because you always know the rate.
 - The velocity v of the reaction is related to the current i , the number of electrons n , and Faraday's constant $F = 96\,485\text{ C/mol e}^-$ via

$$i = nFv$$
 - You can also measure how many product you're forming either by assuming that all current is going to your reaction, or by using in-line gas chromatography.
 - In the EChem module, we'll assume that everything is going to hydrogen evolution.
 - Knowing how much current is going to hydrogen and CO, we can construct a **Tafel plot**.
- **Tafel plot**: The relationship that describes the log-linear dependence of the reaction rate as a function of the applied potential.
 - We will take the partial current going to CO and plot it vs. the applied potential.
 - This yields direct mechanistic insight: Increasing the overpotential decreases the ΔG^\ddagger .
- Example of using a Tafel plot.
 - Assume CO₂ is reduced in a rate limiting step by combining with an electron.
 - Using kinetics, we would have

$$R_{\text{CO}} = k_1(\theta^*)(a_{\text{CO}_2}) \exp\left(\frac{\beta nF}{RT}\right)$$
 - θ^* is the concentration of the active sites on the gold surface; not every atom on the surface is active, as can be shown via fancy microscopy techniques.
 - a_{CO_2} is the **activity** of CO₂ dissolved in solution.
 - β is the symmetry factor: For reactions in which there is a high reorganizational potential energy, we can take $\beta \approx 1/2$.
 - This yields info on the Tafel slope:

$$\frac{\partial \eta}{\partial \log(j)} = \frac{60\text{ mV}}{\beta} = 120 - 150\text{ mV}$$
 - Thus, we check the data: At all potentials in the linear range, check for linear dependence.
 - Tafel data implies ET RLS with slope about 1.
- What if instead, we couple adsorption with proton transfer from?
 - Look at the rate of CO formation vs. the bicarbonate concentration.
 - Nothing here, so it's not this.
 - Moreover, because it's not this charged species, it's not any acidic species (because changes in one would change the pH of all).
 - Nothing for water, too.
 - Thus, the data suggests that there's no proton transfer in the initial step, so it must happen afterwards.

- Note that changing the partial pressure of CO also doesn't change anything, suggesting that as soon as CO is created, it is released and future adsorption is not inhibited.
- Other data complete the mechanism.

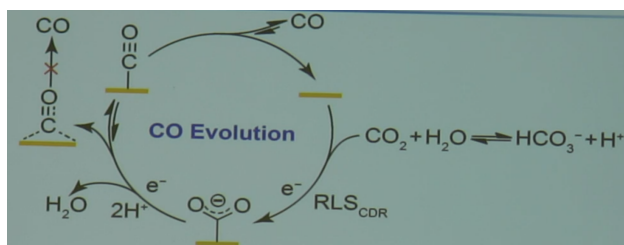
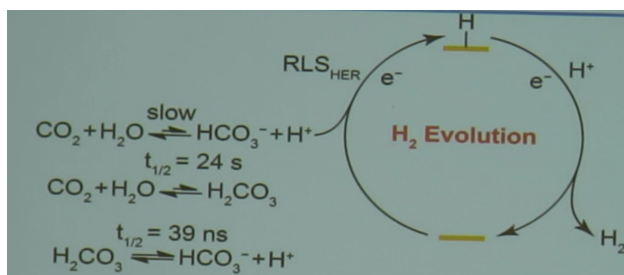
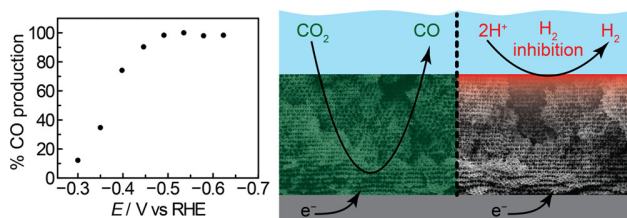


Figure 6.2: CO evolution mechanism.

- Simultaneous hydrogen evolution is dependent on the proton donor environment.

Figure 6.3: H₂ evolution mechanism.

- Mechanism is deceptively simple, but profound all the same.
- We first get adsorption of a proton to a hydride.
 - But Tafel slope is super high, so you may be being limited by the ability of the protons to get to the surface in the first place.
 - Suppose that the protons are special, i.e., donated by the relatively slow dissociation of H₂CO₃.
 - Note that H₂CO₃ dissociates with $t_{1/2} = 24$ s in real life; it is only super fast in our body because of an enzyme we have that takes it to $t_{1/2} = 39$ ns.
 - Changing the concentration of H₂CO₃ and rerunning the experiment confirms this.
- We do observe an explicit change in the rate of hydrogen evolution based on the concentration of H₂CO₃, but the relationship is complex and potential dependent.
- This is an independently occurring catalytic reaction on *some* catalytic site (maybe one that was occupied by CO, maybe not, we don't know).
- Utilizing this mechanism to design a better, more selective reaction.

Figure 6.4: Enhancing heterogeneous CO₂RR with mesoporous membranes.

- If we couple the two reactions, because they both depend on $\text{CO}_2 + \text{H}_2\text{O} \rightleftharpoons \text{HCO}_3^- + \text{H}^+$, we can increase selectivity by slowing down this equilibration even further.
 - We make the environment at the gold catalysis further out of equilibrium with the bulk.
 - Wuttig teamed up with other scientists to develop a mesoporous gold structure, forcing everything that wants to touch the gold to go through the structure.
 - The CO_2 reaction does not care how thick the structure is, but H_2 does! This leads to near-selective CO formation.
- In our module, however, we need to *increase* H_2 evolution, though!
 - We'll use all the same principles Wuttig just discussed, but it'll be simpler.
 - H_2 evolution is also an important reaction.