Lecture #1 of 15

(3: TThF, 5: MT*W*ThF, 4: MT*W*Th, 3: TWTh)

Prof. Shane Ardo
Department of Chemistry
University of California Irvine

Welcome to PHYSICS/CHEM 207!

This course is a recently renamed course at UC Irvine, *with a new-ish instructor = me*!

… thus, while the slides contained in this slide deck were developed last year, they continue to be developed as the course progresses, and so while I cannot tell you how many slides there will ultimately be in this slide deck, what I can tell you is that…

… **It is going to be awesome!**

First… some simple math…

Hey Look! Slides numbers.

Typical UCI 4-unit course

($^5/_6$ hour / lecture class
x 3 class/wk)
+ ($^5/_6$ hour / discussion class
x 1 class/week)
+ ($^5/_6$ hour / office hour "class"
x 1 "class"/week x 20% attendance)
x 10 weeks/quarter
= **35 hours** + 2 hour final exam
= 37 hours/quarter

Our UCI 4-unit summer course:

= (14 days x 3 hours) + (2 days x 2 hours)
= 46 hours/summer
= 2.36 hours / full class + 2 hour final exam

Introductions

Who wants to go first?

… okay, I'll go first…

B.S. in Math (minor in Computer Science)
M.S. in Nutrition
M.A. in (Photo-Physical Inorganic) Chemistry
Ph.D. in (Photo-Physical Inorganic) Chemistry
Post-Doc in Photo-Electro-Chemistry
Professor of Electro- and Photo-Chemistry

… wait, do you know what all those words mean?… they mean what you think they mean… I agree that "Inorganic" is unclear

General Types of Chemists
Makers = **Organic, Inorganic**
Measurers = **Physical**
… but it's not that easy…

Organic = synthesis, polymers, chem bio, etc.

Inorganic = organometallic, synthesis, materials, spectroscopies, etc.

Physical = chemical physics, spectroscopies, computation, analytical, atmospheric, nuclear, etc.

… and this is, of course, also a simplification

Chemical, Applied, and Materials Physics (ChAMP)

… faculty typically associate with at least two of the words that form the ChAMP acronym…

… let's see who they are here: https://champ.uci.edu/faculty/…

… so, as you can imagine, teaching a single cross-disciplinary course to bridge typically siloed departmental foci is not easy… but we're going to try our best to turn each of you into *someone who thinks like a chemist*!…

… thus, we will not cover in great detail nuances of any aspect of chemistry, but we will instead try to share applied chemical concepts that are *likely* most relevant to physicists…

… speaking of which, let's finish up the introductions and I specifically want to know what is the highest level Chemistry course that you have taken (and done moderately well in)…

… okay, let's get started!

Our Tentative Syllabus:

PHYSICS/CHEM 207: Applied Physical Chemistry (http://www.chem.uci.edu/~ardo/applpchem.html)
Departments of Physics & Astronomy / Chemistry, UCI, Summer 2022 *Version Date: 2022.07.04*

Instructor Professor Shane Ardo (ardo@uci.edu); *Office Hours*: By appointment only *(via Zoom)*
Meetings *Class*: M–F @ 9 am – noon PDT (FRH 4135) *(video recordings may be available)*

Course Objectives

- To understand aspects of chemistry that are not often taught to, but are relevant to, physics students
- To instill thermodynamic and kinetic language that unites physics, chemistry, and engineering
- To quantitatively and qualitatively assess chemical systems, experimental data, and problems
- To summarize, explain, and critically evaluate seminal and recent chemistry peer-reviewed articles

Grading *(10% of your lowest score will be dropped)*

50% *Synchronous Assignments* (~10 of them *(your lowest score will be dropped)*; pre-lecture quizzes that will be worked on *individually* and then *in groups* before being submitted)
30% *Asynchronous Final Examination* (*24 hours*; available F7/29 @ 1pm – W8/3 @ 5 pm PDT)
20% *Synchronous Presentation* (*~15 min per student*; during last 1–2 classes (Th7/28 & F7/29))

Course Policies

Late assignments are not accepted, and a make-up examination is not available.
UCI Add/Drop WebReg: https://www.reg.uci.edu/calendars/quarterly/2021-2022/quarterly21-22.html
UCI Chemistry Enrollment Inquiries: https://www.chem.uci.edu/studentaffairs/, or chemistry@uci.edu
UCI Physical Sciences COVID-19 Student Resources: https://uci.edu/coronavirus/students/index.php
UCI Policy on Academic Integrity and Student Conduct: https://aisc.uci.edu/

… this is the bulk of what I propose for the course syllabus…

… thoughts?…

… to start, let's briefly peruse the shell of our course website: https://www.chem.uci.edu/~ardo/applpchem.html

Discussion *(an hour-ish every-other-day-ish)* provides opportunities to discuss applied pchem research…
… of course, there are way too many topics to cover, but I decided on the following as the *tentative* list:

(1) "Single-Molecule Lysozyme Dynamics Monitored by an Electronic Circuit", Y Choi, IS Moody, PC Sims, SR Hunt, BL Corso, I Perez, GA Weiss & PG Collins, *Science*, **2012**, *335*, 319, DOI: 10.1126/science.1214824
(2) "Control of hierarchical polymer mechanics with bioinspired metal-coordination dynamics", SC Grindy, R Learsch, D Mozhdehi, J Cheng, DG Barrett, Z Guan, PB Messersmith & N Holten-Andersen, *Nature Materials*, **2015**, *14*, 1210, DOI: 10.1038/nmat4401
(3) "Experiments and Simulations of Ion-Enhanced Interfacial Chemistry on Aqueous NaCl Aerosols", EM Knipping, MJ Lakin, KL Foster, P Jungwirth, DJ Tobias, RB Gerber, D Dabdub & BJ Finlayson-Pitts, *Science*, **2000**, *288*, 301, DOI: 10.1126/science.288.5464.301
(4) "Potentially Confusing: Potentials in Electrochemistry", SW Boettcher, SZ Oener, MC Lonergan, Y Surendranath, S Ardo, C Brozek & PA Kempler, *ACS Energy Letters*, **2021**, *6*, 261, DOI: 10.1021/acsenergylett.0c02443
(5) "Understanding Multi-Ion Transport Mechanisms in Bipolar Membranes", JC Bui, I Digdaya, C Xiang, AT Bell & AZ Weber, *ACS Applied Materials & Interfaces*, **2020**, *12*, 52509, DOI: 10.1021/acsami.0c12686
(6) "Stable and Efficient Single-Atom Zn Catalyst for CO_2 Reduction to CH_4", L Han, S Song, M Liu, S Yao, Z Liang, H Cheng, Z Ren, W Liu, R Lin, G Qi, X Liu, Q Wu, J Luo & HL Xin, Journal of the American Chemical Society, **2020**, *142*, 12563, DOI: 10.1021/jacs.9b12111
(7) "Visualizing vibrational normal modes of a single molecule with atomically confined light", J Lee, KT Crampton, N Tallarida & VA Apkarian, *Nature*, **2019**, *568*, 78, DOI: 10.1038/s41586-019-1059-9

… whatcha think about these topics?… I'm open to discussing and reconsidering these initial choices…

Our Tentative Syllabus (continued):

Representative Topics Covered

Topic 1 **Chemical Properties** (Molecular nomenclature, Solutions, Balanced chemical reactions, State functions, Standard states, Thermochemistry, Non-ideal gases, Intermolecular forces, Physical properties, Phase changes, Colligative properties, Water activity, Free energy, (X)Chemical potential, Chemical equilibrium, van't Hoff equation, Activity coefficients, Le Chatelier's principle, Schrödinger equation, Atomic orbitals, Hybridization, Valence bond theory, Molecular orbital theory, Band diagrams, Crystal field theory, Ligand field theory)

Topic 2 **Charged Interfaces** (Redox half-reactions, Nernst equation, Electrodes, Potentiostat, Pourbaix diagram, Electric potential, Double layer, Membrane potential, Liquid-junction potential, Donnan potential, Acidity scale, pH probe)

Topic 3 **Chemical Kinetics** (Continuity of mass, Mass transfer, Nernst–Planck equation, Diffusion, Diffusion coefficient, Migration, Mobility, Convection, Boundary layer, Mass action, Microscopic reversibility, Förster cube, Square schemes, Activation energies, Marcus–Hush theory, Transition-state character, Reorganization energy, Linear free energy relationships, Superexchange, Outer/inner sphere, Butler–Volmer equation, Fermi's golden rule, Solid-state physics, Gerischer theory, Rate-determining step, Steady-state/Pre-equilibrium approximations, Langmuir/Frumklin isotherms)

Topic 4 **Photochemistry** (Blackbody radiation, Einstein coefficients, Born–Oppenheimer approximation, Harmonic oscillator model, Franck–Condon principle, Transition dipole moment operator, Beer–Lambert law, Absorption coefficient, Oscillator strength, Absorptance, Jablonski diagram, Internal conversion, Intersystem crossing, Thexi state, Kasha–Vavilov rule, Luminescence processes, Conservation laws, Selection rules, E–k diagrams, Energy transfer processes, Excited-state photochemical reactions, Photochemical length scales, Photochemical time scales, Electromagnetic spectrum, Steady-state spectroscopies, Pump–probe transient spectroscopies)

… this is the proposed Coursework Plan…

… Assignments are Quizzes, but do not fear, they are Group Quizzes!…

… at the start of each class, you will **take a Quiz alone**…

… then you will split up into small groups to converge on answers and **submit a Group Quiz assignment** to Canvas…

… then we will **discuss the Quiz problems** as a class…

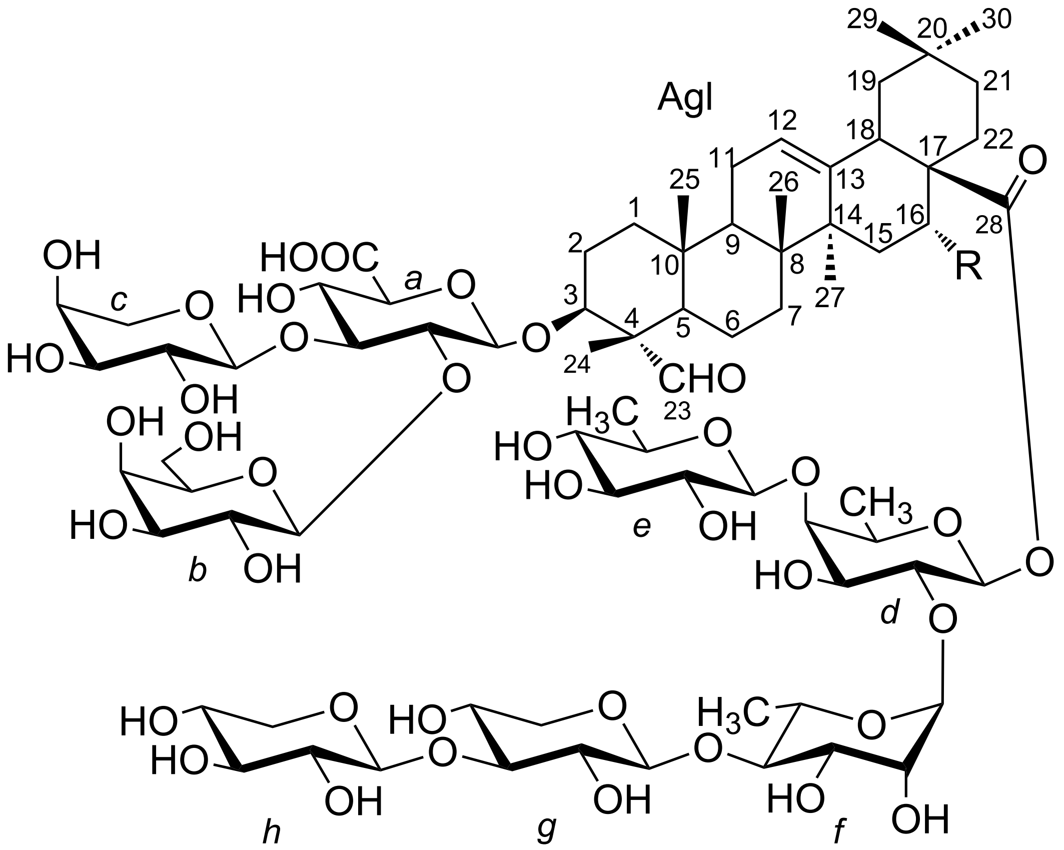
… for your Final Exam, know how to answer the Quiz problems… wink, wink!

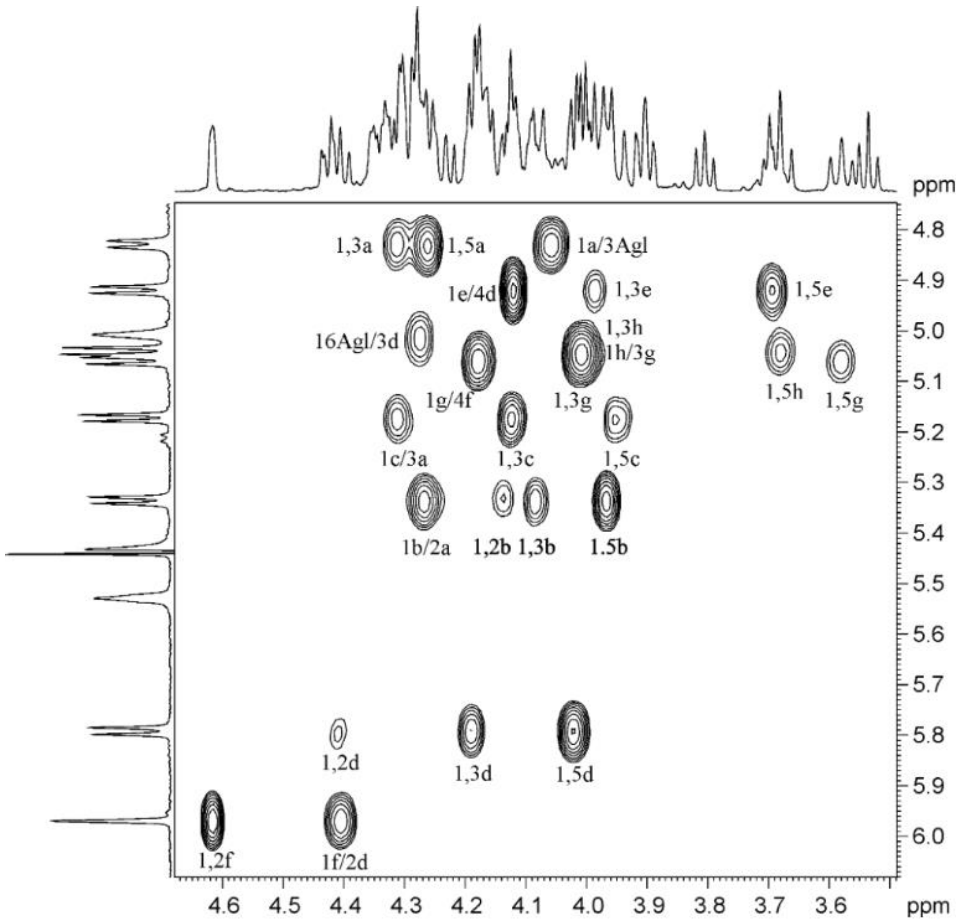
Q: What differentiates chemistry from physics?

A: That is a tough question… Wiki provides some reasonable interpretations…

… https://en.wikipedia.org/wiki/Chemistry#Modern_principles

Example: knowing how every atom is bonded and arranged in a complex molecule





https://www.beilstein-journals.org/bjoc/articles/8/87

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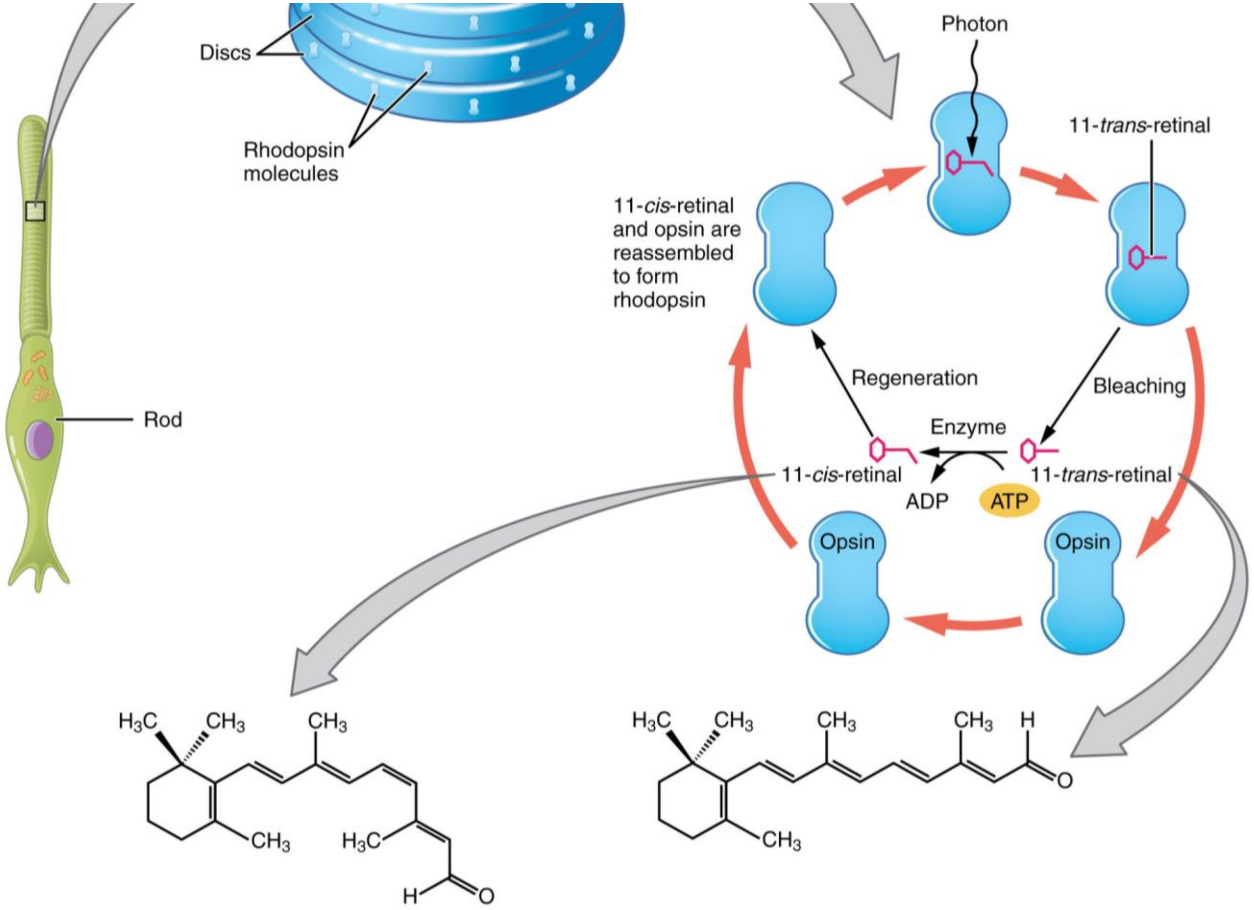
Example: absorption of a photon results in bending of a molecule as human vision



https://en.wikipedia.org/wiki/Visual_phototransduction#/media/File:1415_Retinal_Isomers.jpg

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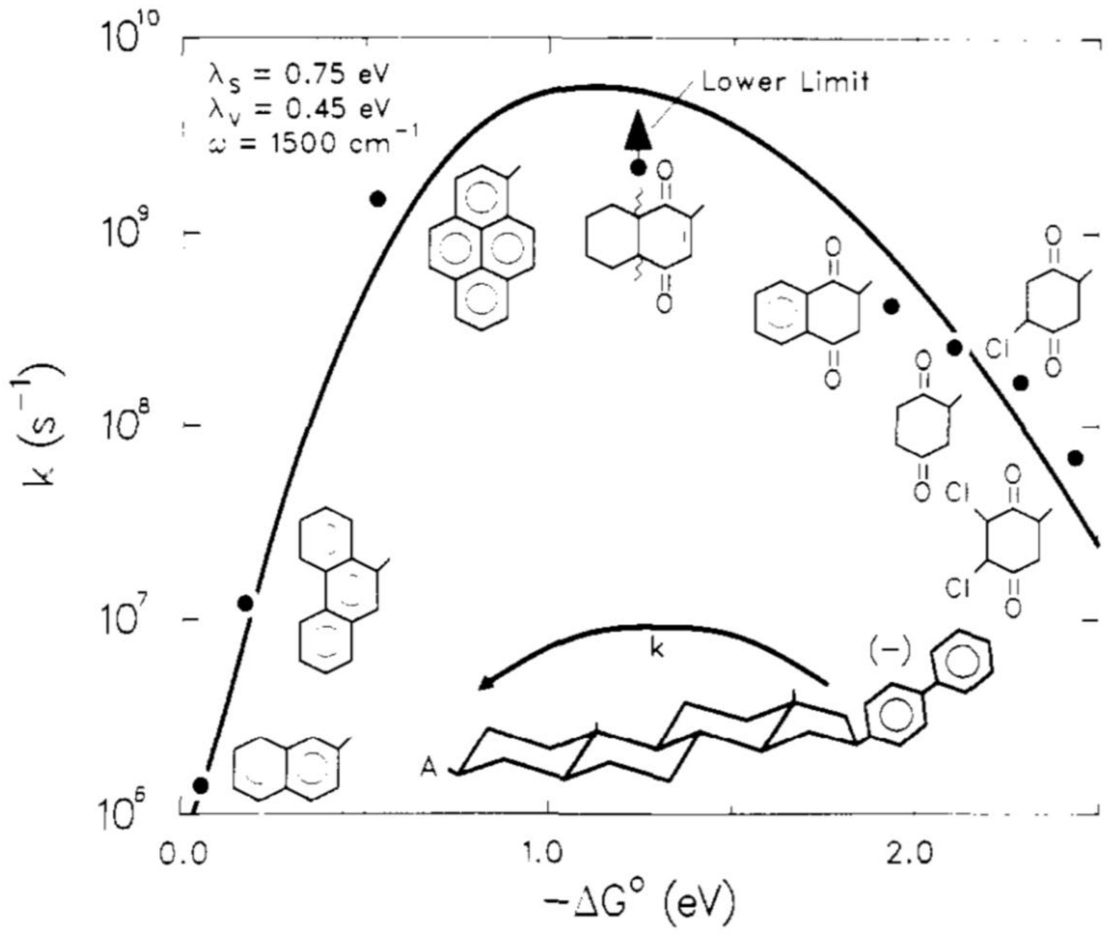
Example: electron-transfer rates in solution slow when highly thermodynamically favored



https://pubs.acs.org/doi/abs/10.1021/ja00322a058

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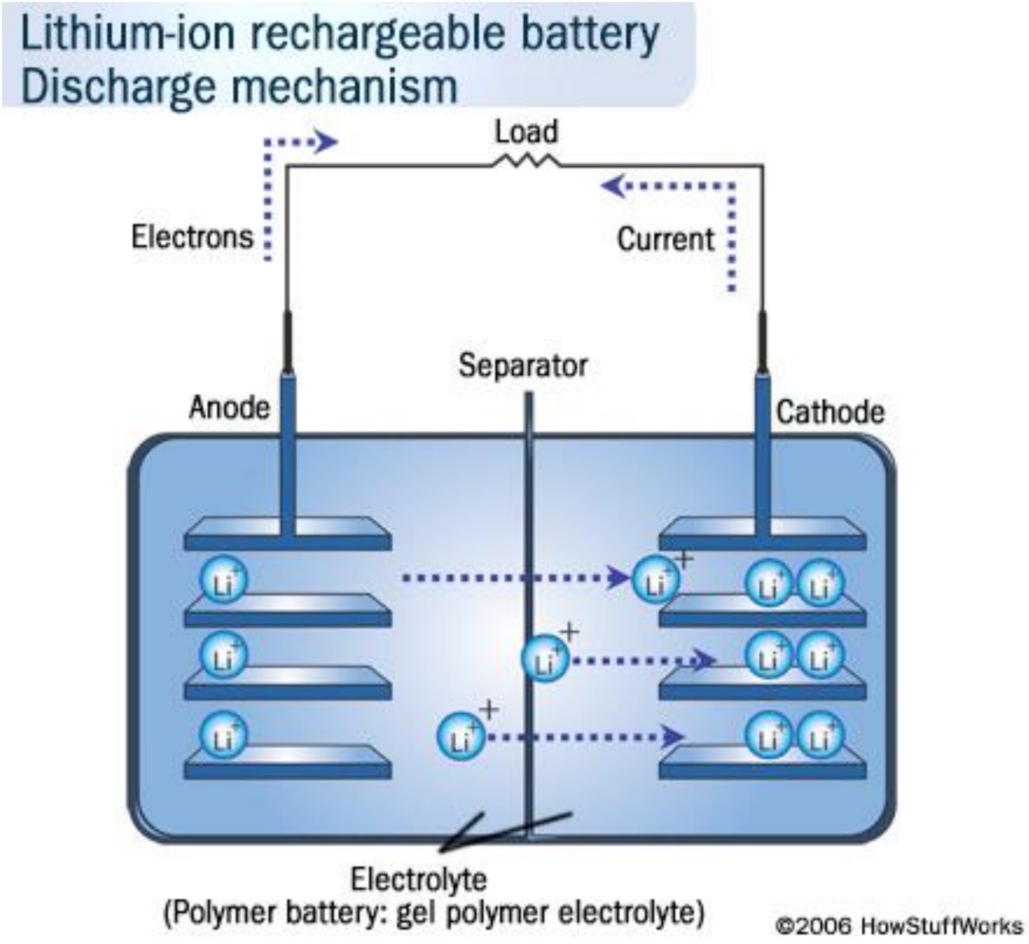
Example: rechargeable batteries

Nobel Prize in Chemistry in 2019!
https://www.nobelprize.org/prizes/chemistry/2019/press-release/

http://www.evworld.com/images/a123_csize.jpg



http://auto.howstuffworks.com/fuel-efficiency/vehicles/lithium-ion-battery-car1.htm

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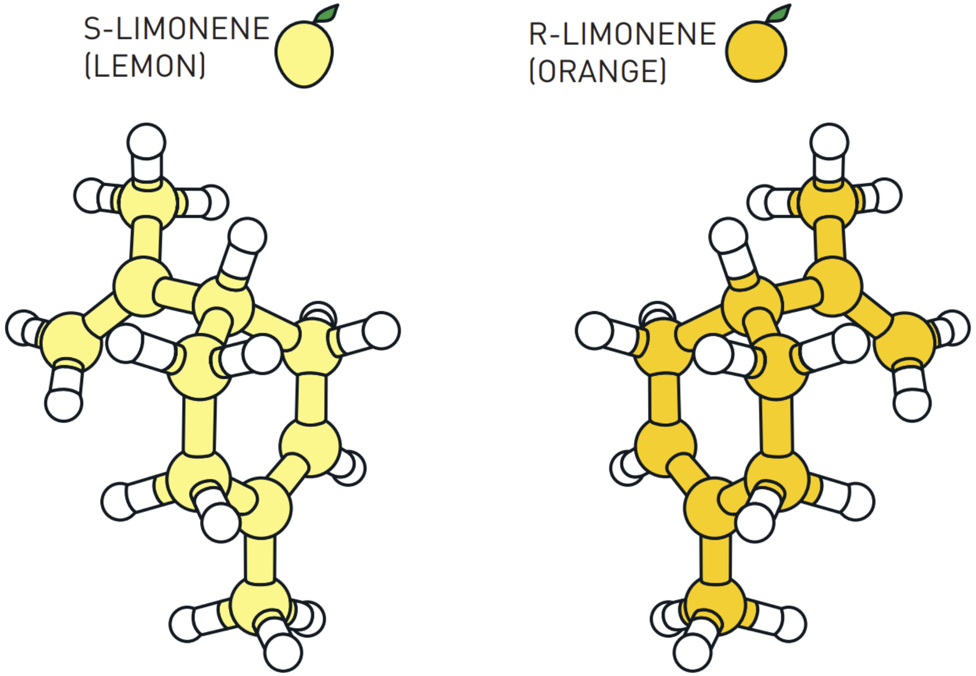
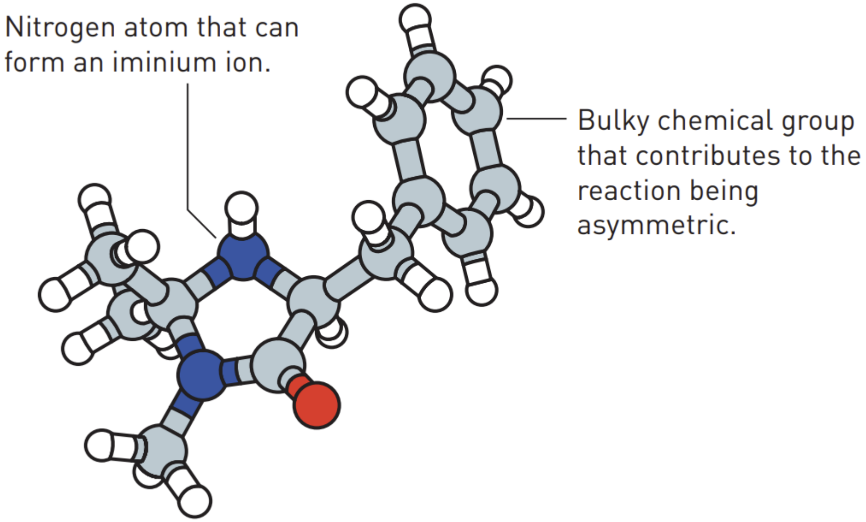
Example: asymmetric organocatalysis

Nobel Prize in Chemistry in 2021!

https://www.nobelprize.org/prizes/chemistry/2021/press-release/



enantiomers



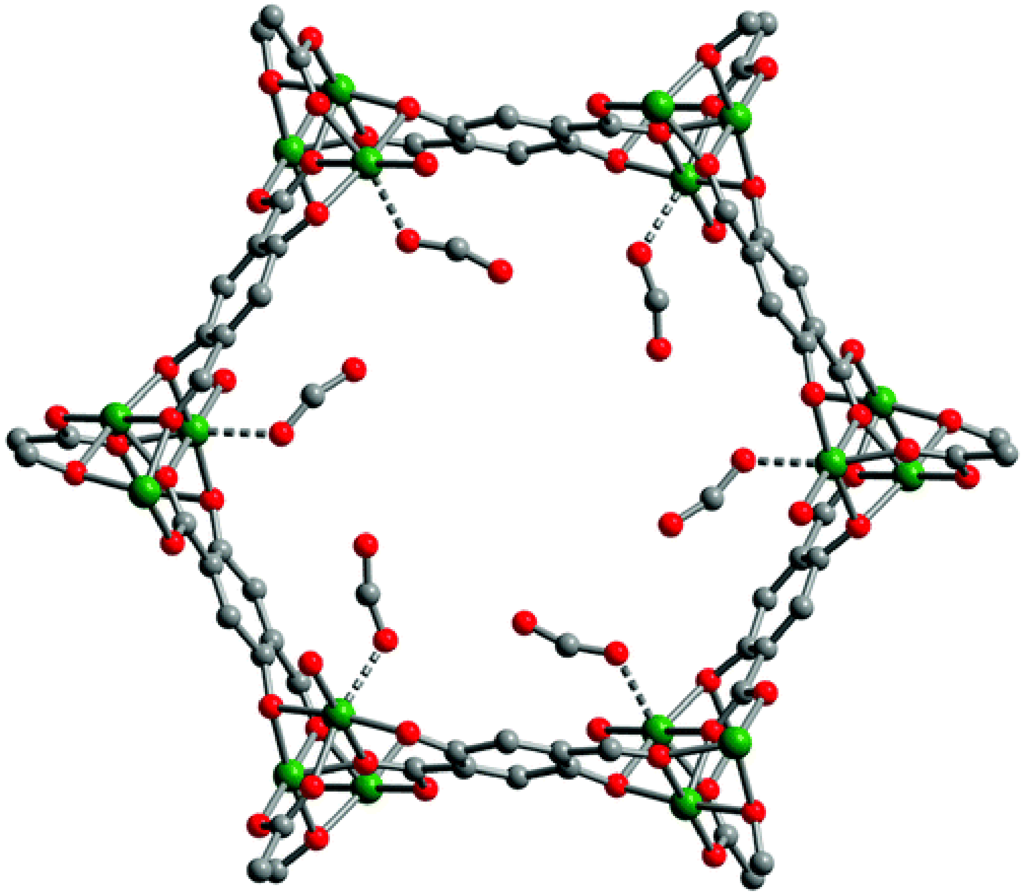
2 He designed some simple molecules that could create iminium ions. One of these proved to be excellent at asymmetric catalysis.

Q: What differentiates chemistry from physics?

A: That is a tough question… Wiki provides some reasonable interpretations…

… https://en.wikipedia.org/wiki/Chemistry#Modern_principles

Example: capture of CO_2 from air in atomically precise metal–organic framework



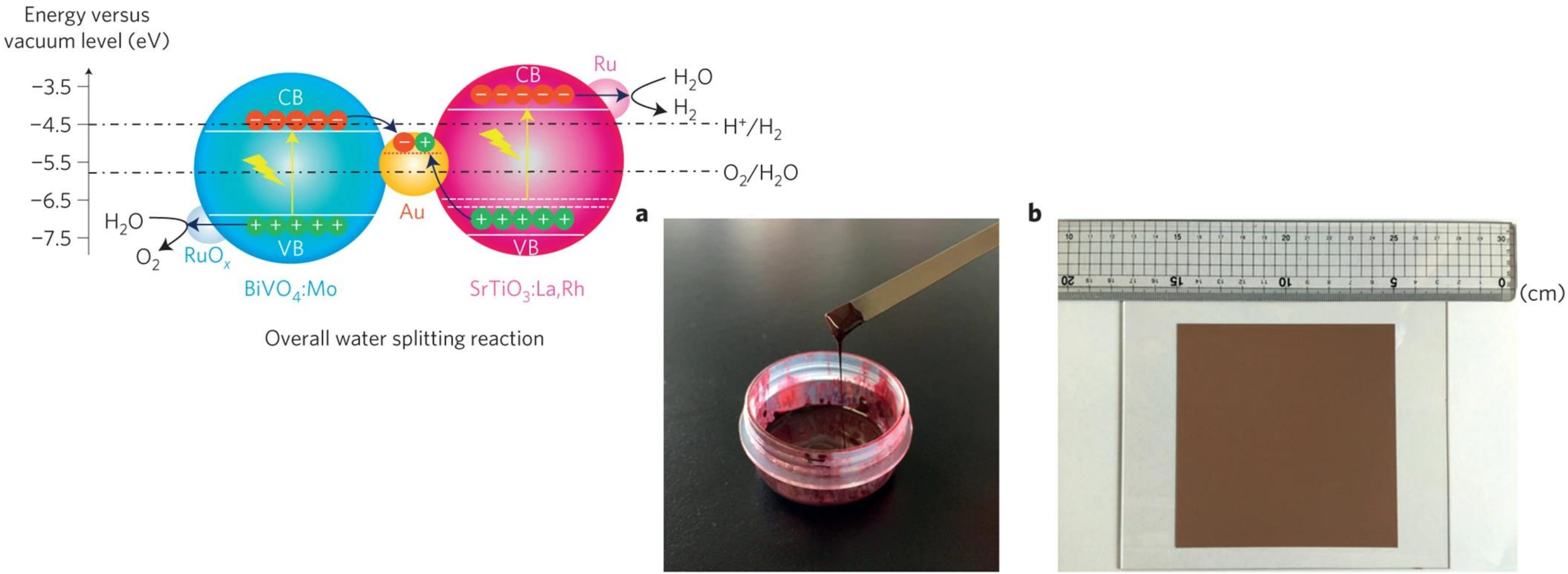
https://www.nature.com/articles/nmat4589

Q: What differentiates chemistry from physics?

A: That is a tough question… Wiki provides some reasonable interpretations…

… https://en.wikipedia.org/wiki/Chemistry#Modern_principles

Example: shining sunlight on five-component paint immersed in water evolves H_2 and O_2



https://www.nature.com/articles/nmat4589

Q: What differentiates chemistry from physics?

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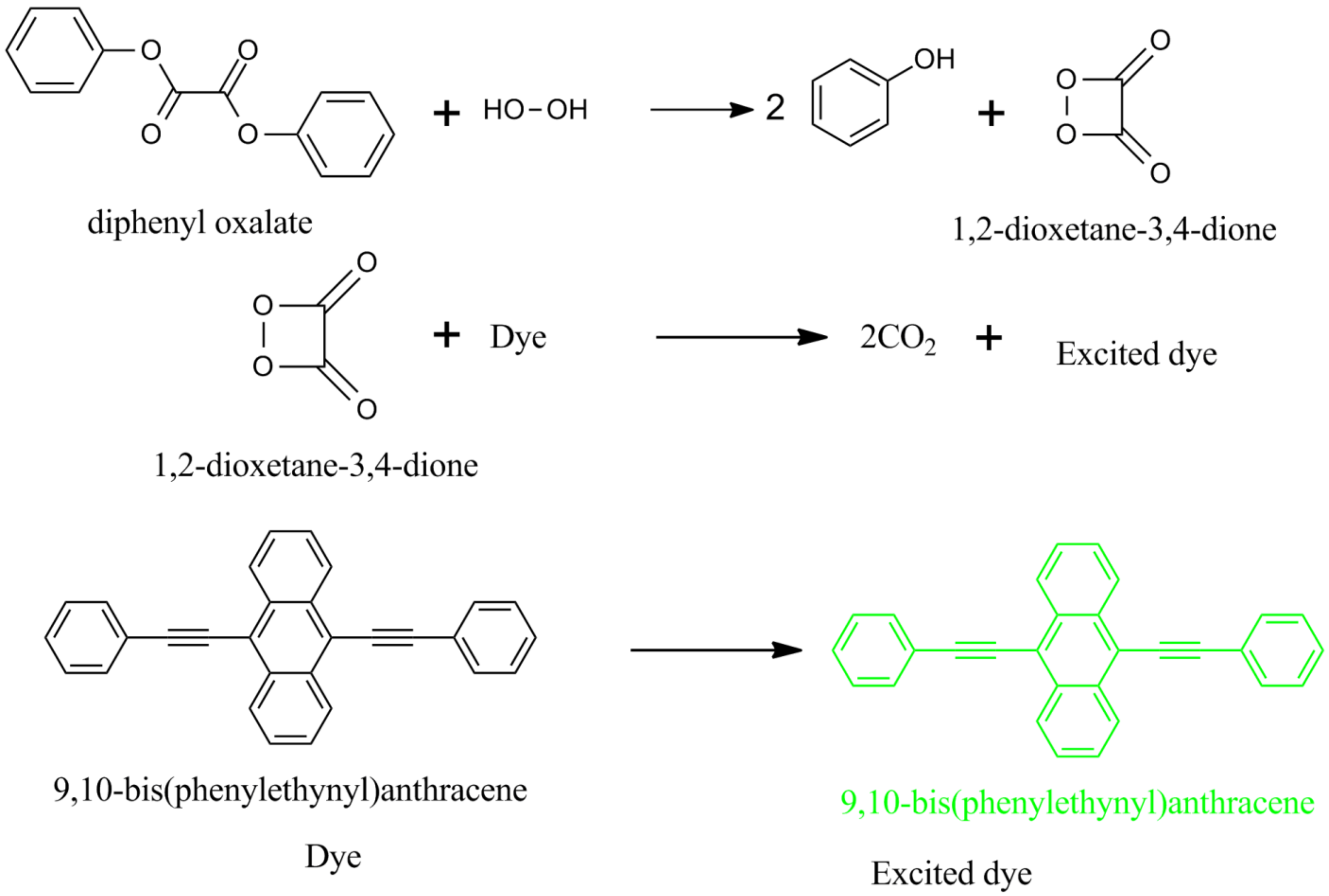
… https://en.wikipedia.org/wiki/Chemistry#Modern_principles

Example: glowstick chemiluminescence



https://glitchmind.com/scorpions-glow-beautifully-under-uv-light/

so we can already conclude that chemistry…

… is super cool… but you already knew that…

… is quite diverse, and thus requires a wide range of knowledge

… is at the heart of some very interesting, and still unexplained, scientific observations

… opens up many opportunities to innovate on new processes and technologies

… and is consequently an extremely active area of scientific endeavor, of course!

Course philosophy (me *versus* you)

Theory/Experiments *versus* Applications/Processes

I will teach the theory, history, and experimental specifics, and you will teach details of the applications and interesting recent chemical discoveries

… wow, those were some neat examples of chemistry…

… I wish I could learn more about all of them!

… Lucky you! … Lucky us!

- Synchronous presentation: 12 min max + 3 min for Q&A, as 6 – 8 slides *emailed to me the day before the presentation*

- One seminal and/or review publication (~70% of the time); include background and the nitty gritty of how it works; **your main goal should be to bridge information presented in the course to your topic, and to teach us something entirely new related to *chemistry***

- One recent publication (2015 or later) (~30% of the time); include what the paper did, the major discovery, and a critical chemical assessment of their data interpretation, **including at least one graph or plot of useful *chemical* data**!

… this, plus the Assignments, equal 70% of your course grade, so take them seriously, and HAVE FUN!

e-Presentation… *to get a general idea, these are good topic choices in photo-chemistry alone*…

- silver-halide photography
- photolithography
- vision
- vitamin D synthesis
- ultraviolet-light-driven DNA dimerization
- natural photosynthetic ion pump
- natural photosynthetic light-harvesting complex and coherent energy transfer
- natural photosynthetic Z-scheme electron-transport chain
- nanoparticle solar fuels photocatalysis
- dye-sensitized solar cells
- excitonic solar cells with trap states
- dye lasers
- medical applications
- fluorescence microscopy pH sensing
- fluorescence microscopy electric field sensing
- long-lived phosphorescence by organic molecules
- persistent luminescence by lanthanide-doped phosphors
- chemiluminescence
- photoredox catalysis in organic synthesis
- photolabile organic radicals
- atmospheric chemistry in the ozone layer with refrigerants
- photolabile inorganic coordination compounds
- light-induced excited spin-state trapping (LIESST) spin-crossover effect
- molecular solar thermal energy storage (MOST)
- triplet-triplet annihilation upconversion
- hot/ballistic excited-state electron transfer

… or propose your own to me… which I really do prefer that you do

… you will get one of your top 5 choices… more info coming soon…

e-Presentation… *and these are good topic choices in electro-chemistry alone*…

- fast electrochemistry
- low conductivity electrochemistry
- rotating (ring) disk electrochemistry
- electro-osmotic flow
- electrochemical impedance spectroscopy
- bulk (water) electrolysis
- thin-layer electrochemistry
- stripping analysis
- coupled reactions / catalysis
- modified electrodes
- electrochemical scanning tunneling microscopy
- scanning electrochemical microscopy
- spectroelectrochemistry
- in situ, operando spectroscopy
- electrochemical quartz crystal microbalance
- electro-generated chemiluminescence
- aluminum extraction and processing
- bipolar electrochemistry
- electrodeposition / electroless deposition
- chlor-alkali process
- polymer-electrolyte fuel cells
- solid-oxide fuel cells / electrolyzers
- batteries (acid/base; intercalation)
- redox flow batteries
- electrochemical supercapacitors
- (bio)sensors
- electrodialysis
- nanopore/nanorod ion conductors

… or propose your own to me… which I really do prefer that you do

… you will get one of your top 5 choices… more info coming soon…

okay, so that ends the introduction to the course…

… before we get started, let's agree on the course format…

… then let's agree that we should take a break somewhat soon…

… but before – or after – we do, let's take a **quick quiz** (Assignment) on the alphabet of physical chemistry!… it's on our Canvas website under Files… if need be, you can use the Internet to help you, but if you do, please indicate it on the quiz…

… when you are finished, upload your quiz in any format that you desire to our Canvas website under Assignment 1…

… then let's break up into small groups to get on the same page… one person should also upload your group work to our Canvas website under Assignment 1 – GROUPS…

… and finally we'll come back together to see how that worked and discuss further

Chemical Properties

Prof. Shane Ardo
Department of Chemistry
University of California Irvine

Chemical Properties

- **Molecular nomenclature, Solutions, Balanced chemical reactions**
- **State functions, Standard states, Thermochemistry**
- Non-ideal gases, Intermolecular forces, Physical properties, Phase changes, Colligative properties, Water activity
- Free energy, (X)Chemical potential, Chemical equilibrium, van't Hoff equation, Activity coefficients, Le Chatelier's principle
- Schrödinger equation, Internal energy, Atomic orbitals, Hybridization
- Valence bond theory, Molecular orbital theory, Band diagrams
- Crystal field theory, Ligand field theory

Great online resource: http://www.rnlkwc.ac.in/pdf/study-material/chemistry/Peter_Atkins__Julio_de_Paula__Physical_Chemistry__1_.pdf

Physical Properties of Chemicals

… so what is the best way to do this quickly… as it's just as painful for me as it is for you?…
… I have an idea!…

… Wikipedia!… but how do we choose a chemical to look up?… I have another idea!…

… let's see what's in that COVID-19 vaccine:
https://www.hackensackmeridianhealth.org/HealthU/2021/01/11/a-simple-breakdown-of-the-ingredients-in-the-covid-vaccines/
… let's first try with ethanol: https://en.wikipedia.org/wiki/Ethanol
… then let's try 2-hydroxypropyl-β-cyclodextrin: https://en.wikipedia.org/wiki/Cyclodextrin
… and finally, what about 1,2-distearoyl-snglycero-3-phosphocholine [DSPC]:
https://en.wikipedia.org/wiki/Distearoylphosphatidylcholine… Wow!

… on another note, how about sunscreen?… welcome to SoCal!:
https://www.aad.org/public/everyday-care/sun-protection/shade-clothing-sunscreen/is-sunscreen-safe… This is fun!… Let's not stop!… Okay, let's stop…

Solutions and Concentration

Concentration can be expressed in terms of molarity (M), molality (m), and fractions (X, w)…

… yes, seriously!

$$M = \frac{\text{moles of solute}}{\text{volume of solution}}$$

Units: ***M* = mol L^{-1}**

Also used: m*M*, n*M*, …

… most common!

$$m = \frac{\text{moles of solute}}{\text{kg of solvent}}$$

Units: ***m* = mol kg^{-1}**

$$X = \frac{\text{moles of solute}}{\text{moles of solute + solvent}}$$

Unitless

$$w = \frac{\text{kg of solute}}{\text{kg of solution}}$$

Unitless

sometimes expressed in:
wt% = *w* x 100
ppm = *w* x 10^6

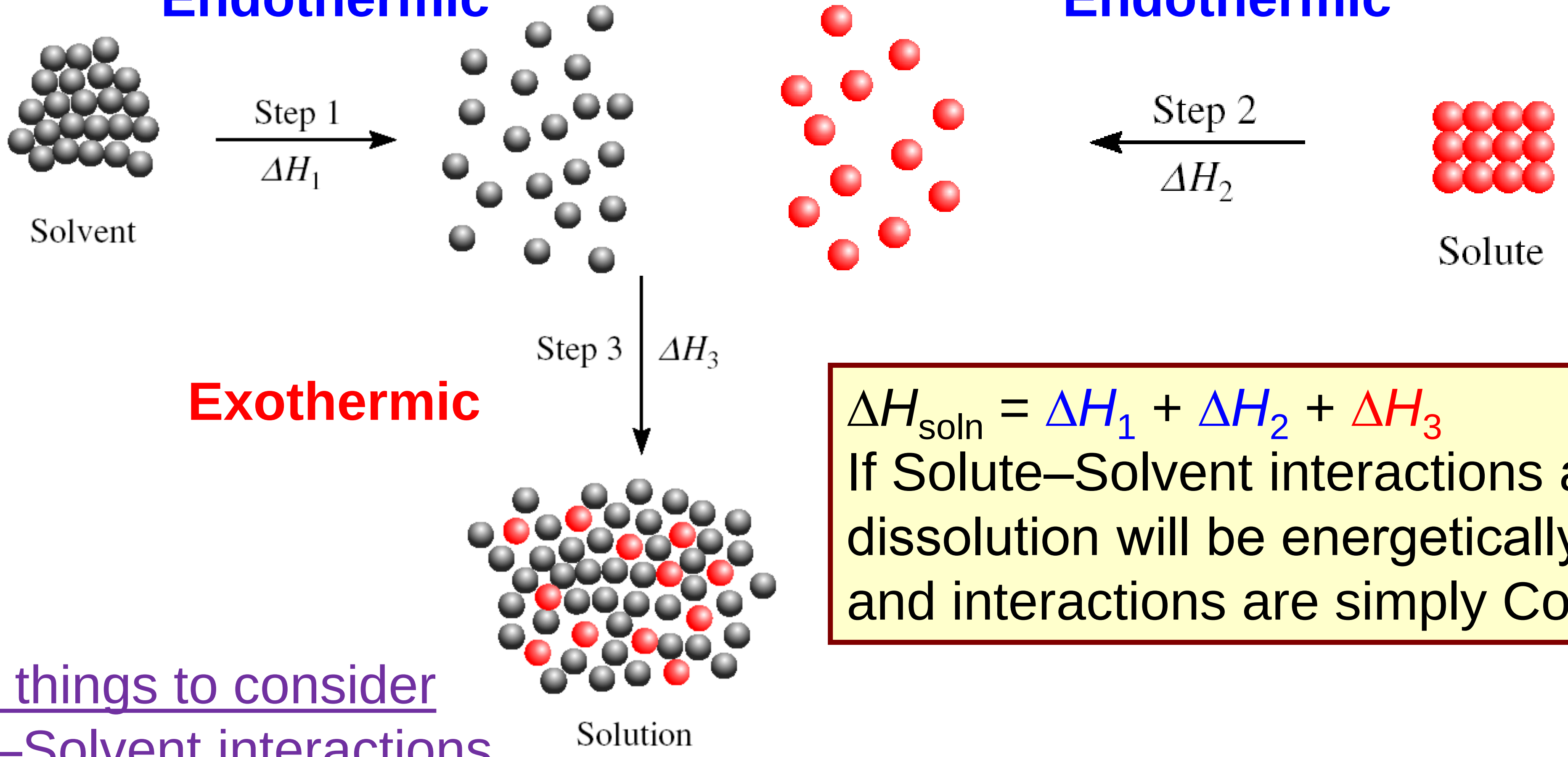
Solution – **homogenous** (uniform) mixture of two or more chemical components

Solute – component present in the smaller amount

Solvent – component present in the larger amount

Molecular View of Dissolution

Endothermic **Endothermic**



Exothermic

$\Delta H_{soln} = \Delta H_1 + \Delta H_2 + \Delta H_3$

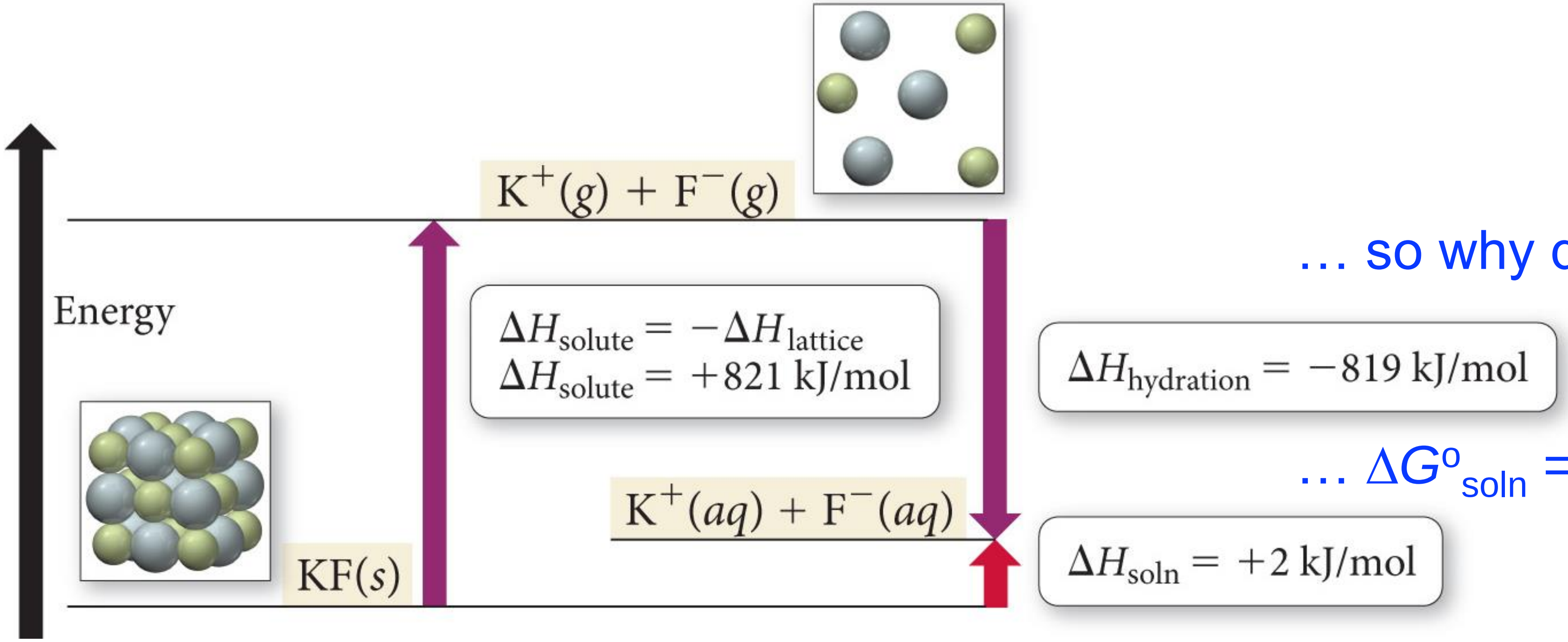
If Solute–Solvent interactions are strong, dissolution will be energetically favored… and interactions are simply Coulombic!

<u>Important things to consider</u>

- Solvent–Solvent interactions
- Solute–Solute interactions
- Solvent–Solute interactions

Have you ever heard of the hydrophobic effect?
… it requires this kind of chemical thinking…

Thermochemistry of Dissolution



… so why does the reaction occur?

… $\Delta G^o_{soln} = \Delta H^o_{soln} - T\Delta S^o_{soln}$!

What is ΔG^o?… and ΔG?

What do I feel when I hold the beaker?

Lattice energy: $KF(s) \rightarrow K^+(g) + F^-(g)$

Hydration energies: $K^+(g) \rightarrow K^+(aq)$ and $F^-(g) \rightarrow F^-(aq)$

Dissolution energy: $KF(s) \rightarrow K^+(aq) + F^-(aq)$

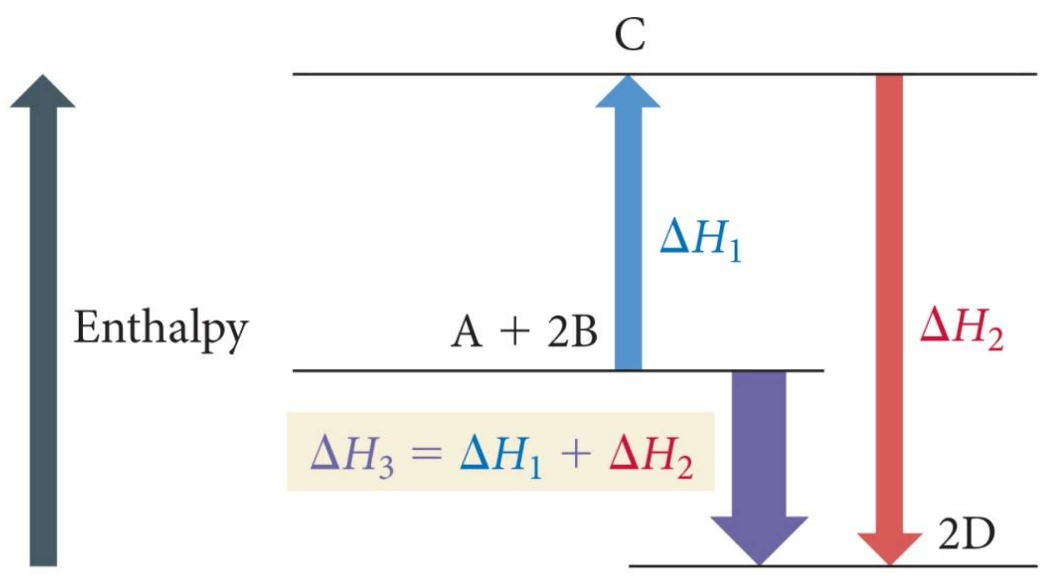
Endothermic ($\Delta H^o_{soln} > 0$) because $|\Delta H^o_{lattice}| > |\Delta H^o_{hydration}|$

Series of Chemical Reactions

If a reaction can be expressed as a series of steps, then the ΔH_{rxn} for the overall reaction is the sum of the heats of reaction for each step

Hess's Law

The change in enthalpy for a stepwise process is the sum of the enthalpy changes of the steps.



… but why is this the case?

… is change in enthalpy the only property that follows this rule?

… does change in enthalpy dictate whether this reaction occurs or not? If not, what does?

A + 2B → C
<u>C → 2D</u>
A + 2B → 2D

Balancing Reactions

$C_6H_4(OH)_2$ (aq)	$\longrightarrow$	$C_6H_4O_2$ (aq) + H_2 (g)	ΔH = +177.4 kJ/mol
H_2 (g) + O_2 (g)	$\longrightarrow$	H_2O_2 (aq)	ΔH = –191.2 kJ/mol
H_2 (g) + $\frac{1}{2}O_2$ (g)	$\longrightarrow$	H_2O (g)	ΔH = –241.8 kJ/mol
H_2O (g)	$\longrightarrow$	H_2O (l)	ΔH = –43.8 kJ/mol

Use measured reaction enthalpies to calculate ΔH for the following reaction:

$$C_6H_4(OH)_2\ (aq) + H_2O_2\ (aq) \longrightarrow C_6H_4O_2\ (aq) + H_2O\ (l)$$

1. Balance the chemical equation.

What is this missing?

2. Reorder the sub-reactions with reactants to the left and products to the right, and correct for stoichiometries.

$C_6H_4(OH)_2$ (aq)	$\longrightarrow$	$C_6H_4O_2$ (aq) + H_2 (g)	ΔH_1 = +177.4 kJ/mol
H_2O_2 (aq)	$\longrightarrow$	H_2 (g) + O_2 (g)	ΔH_2 = – (–191.2) kJ/mol
$2H_2$ (g) + O_2 (g)	$\longrightarrow$	$2H_2O$ (g)	ΔH_3 = 2×(–241.8) kJ/mol
$2H_2O$ (g)	$\longrightarrow$	$2H_2O$ (l)	ΔH_4 = 2×(–43.8) kJ/mol
$C_6H_4(OH)_2$ (aq) + H_2O_2 (aq)	$\longrightarrow$	$C_6H_4O_2$ (aq) + $2H_2O$ (l)	

Assuming that this overall reaction is spontaneous ($\Delta G < 0$), and we had 1 mol of each species, which species is the limiting reagent?

What do I feel when I hold the beaker?

3. Do some arithmetic.

$$\Delta H = \Delta H_1 + \Delta H_2 + \Delta H_3 + \Delta H_4 = 177.4 + 191.2 - 483.6 - 87.6 = -202.6 \text{ kJ/mol}$$

Standard States

To define a thermochemical state of a (chemical) system, one needs boundary conditions!

For an element, standard *chemical* practice is to use:

The most stable state in which the element exists under conditions of p = 1 atm and T = 25 °C

For a compound, standard *chemical* practice is to use:

Gaseous substance: p = 1 atm and T = 25 °C

Liquid or solid substance: pure liquid or solid

Substance in solution: 1 M solution

If more than one form of the element exists under the standard conditions, use the most stable form

⇨ Oxygen (g) can exist as O_2 or as O_3 (ozone) at 1 atm and 298 K

Most stable form = O_2 (g)
ΔH_f^o = 0 kJ/mol

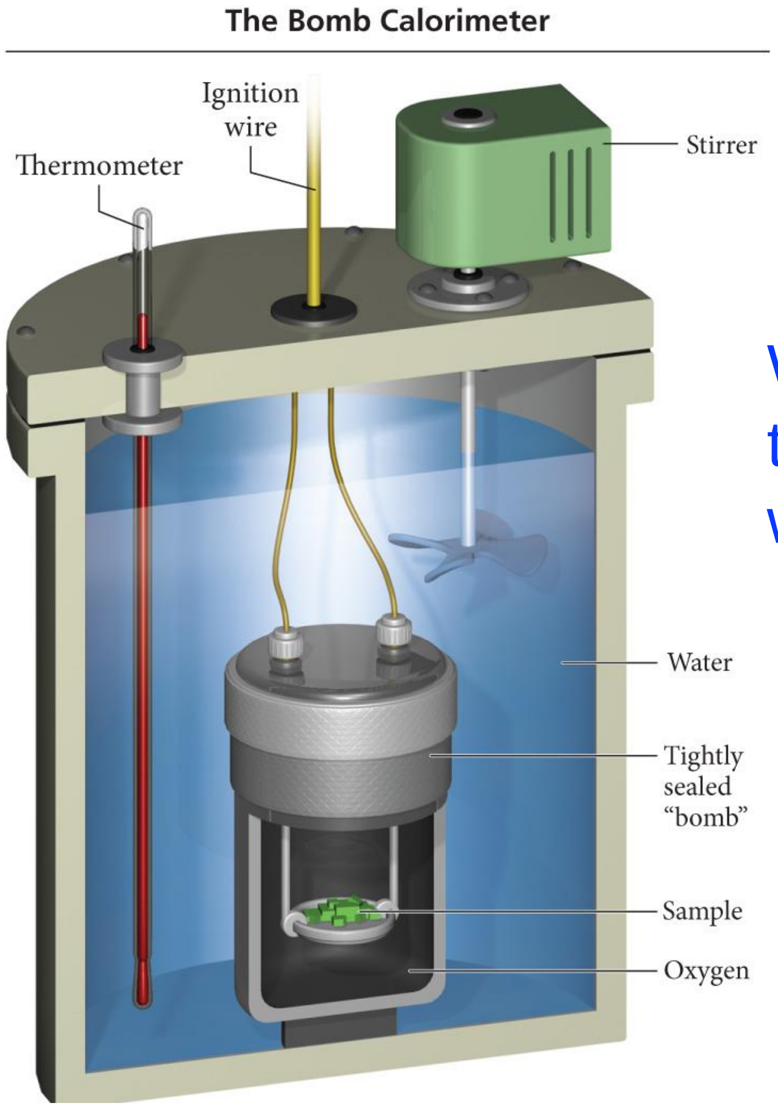
Less stable form = O_3 (g)
ΔH_f^o = +142.7 kJ/mol

⇨ Carbon (s) can exist as graphite or as diamond at 1 atm and 298 K

Most stable form = graphite ΔH_f^o = 0 kJ/mol

Less stable form = diamond ΔH_f^o = +1.88 kJ/mol

Measuring Changes in Internal Energy or Enthalpy

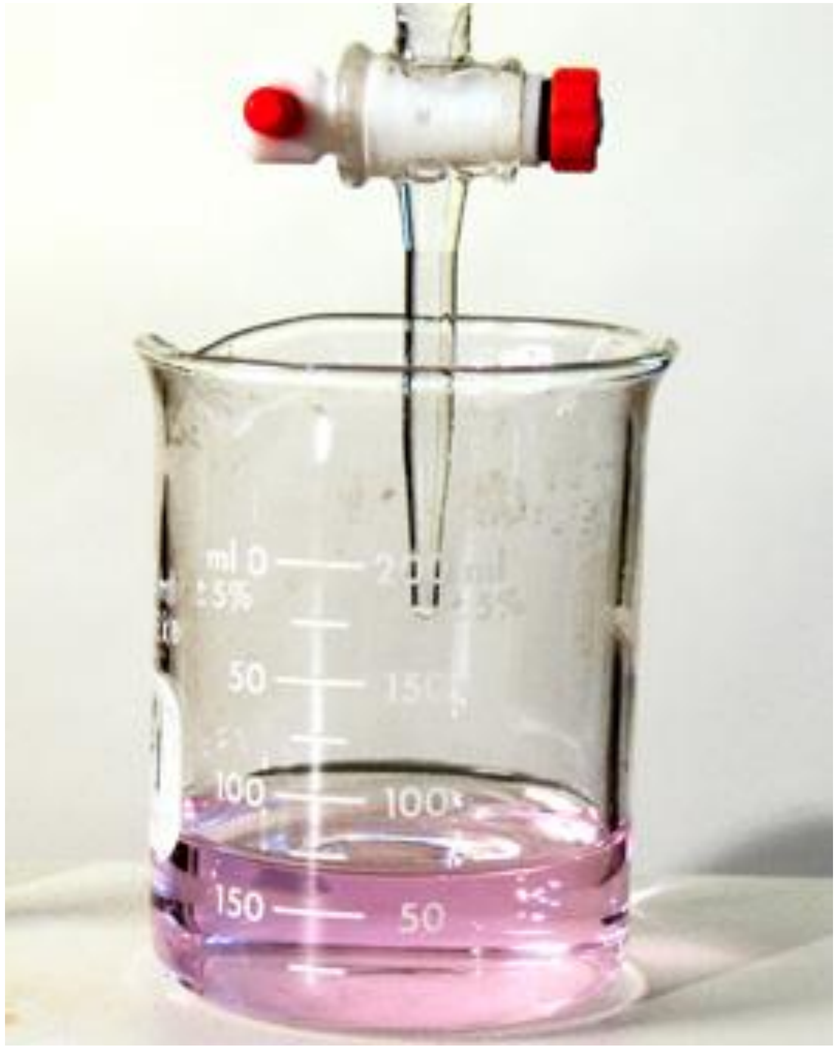


Which should we use to measure ΔE, and which to measure ΔH?

Does this help?

$\Delta E = q_v = C_v \Delta T$

$\Delta H = q_p = C_p \Delta T$



Chemical Properties *(summary for today)*

- **Molecular nomenclature, Solutions, Balanced chemical reactions**
- **State functions, Standard states, Thermochemistry**
- Non-ideal gases, Intermolecular forces, Physical properties, Phase changes, Colligative properties, Water activity
- Free energy, (X)Chemical potential, Chemical equilibrium, van’t Hoff equation, Activity coefficients, Le Chatelier’s principle
- Schrödinger equation, Internal energy, Atomic orbitals, Hybridization
- Valence bond theory, Molecular orbital theory, Band diagrams
- Crystal field theory, Ligand field theory