Exploring the Current Applications and Research of General Chemistry Topics

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Outline

- Unit-by-unit examples
  - Real-world application
  - Current research
  - Collaborate!
- Resources

AP Chemistry (2022-2023)

Unit 1: Atomic Structure and Properties
Unit 2: Molecular and Ionic Compound Structure and Properties
Unit 3: Intermolecular Forces and Properties
Unit 4: Chemical Reactions
Unit 5: Kinetics
Unit 6: Thermodynamics
Unit 7: Equilibrium
Unit 8: Acids and Bases
Unit 9: Applications of Thermodynamics

Unit 1: Atomic Structure & Properties

UNIT 1 Atomic Structure and Properties

~9–10 Class Periods | 7–9% AP Exam Weighting

SPQ 5	1.1	Moles and Molar Mass
SPQ 5	1.2	Mass Spectroscopy of Elements
SPQ 2	1.3	Elemental Composition of Pure Substances
SPQ 5	1.4	Composition of Mixtures
SAP 1	1.5	Atomic Structure and Electron Configuration
SAP 4	1.6	Photoelectron Spectroscopy
SAP 4	1.7	Periodic Trends
SAP 4	1.8	Valence Electrons and Ionic Compounds

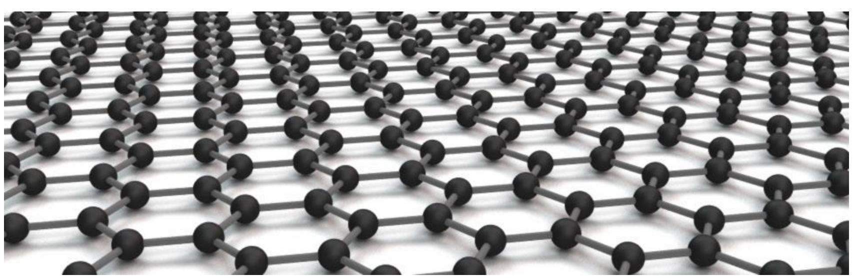
- Visualizing the Atom: TEM
- Measuring Orbitals in Quantum Mechanical Model
  - XPS – core electrons
  - UPS – valence electrons
- General Applications of Isotopes

How do we know atoms exist?

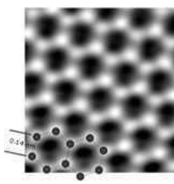
Atom: smallest particle of an element that retains its chemical identity

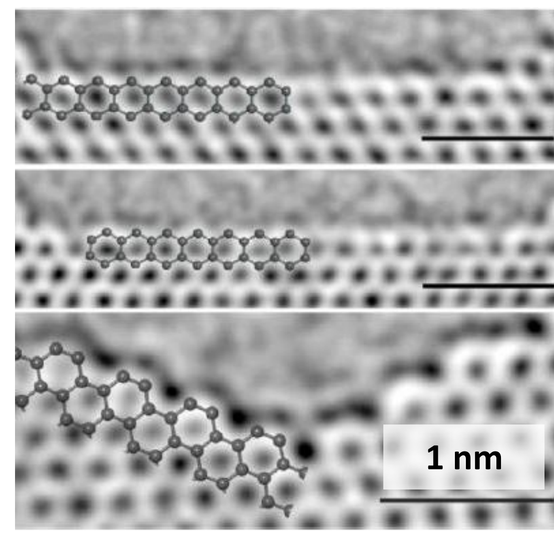
- How do we know it exists?
- Can we see it?

Graphene: a single layer of graphite



Transmission Electron Microscope images of graphene

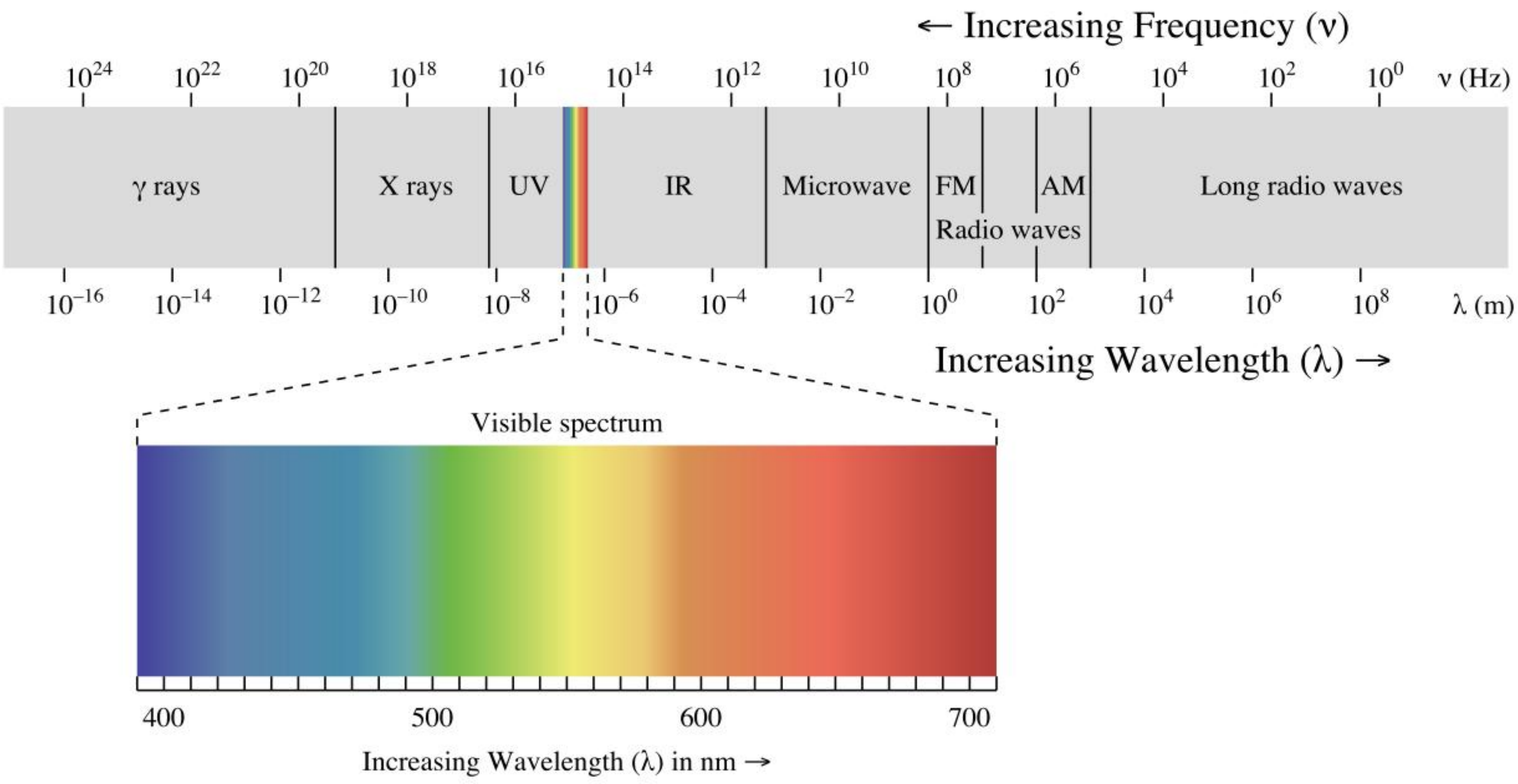




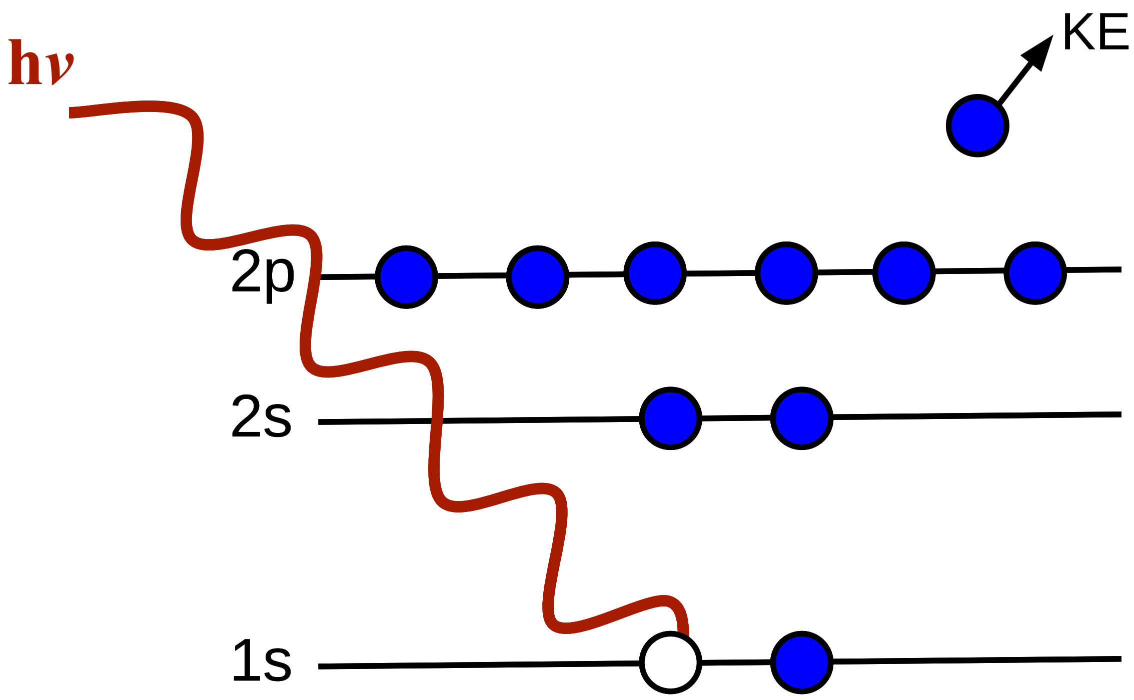
Sur, U. *Inter J of Electrochem*. (2012) 10.1155/2012/237689.
H. Kuang, et al, *ACS Nano* (2015) 9, 5, 4786–4795.

How do we measure energy of electrons in orbitals?

X-ray and Ultraviolet photoemission spectroscopy



How do XPS & UPS work?



XPS
- Study core electrons

UPS:
- Study valence electrons

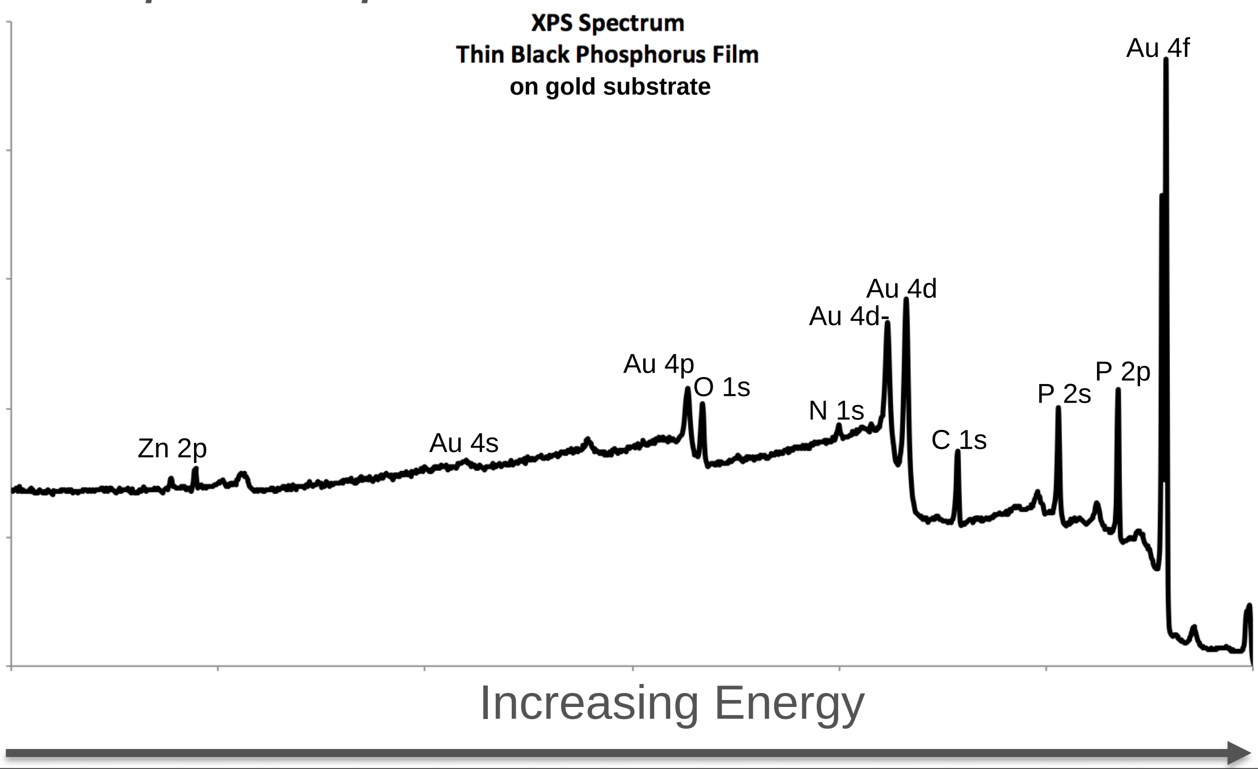
XPS of Phosphorus on Gold

Phosphorus, P

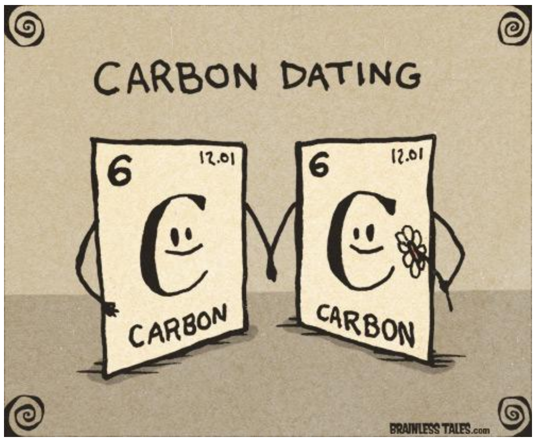
- Electron configuration: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^3$

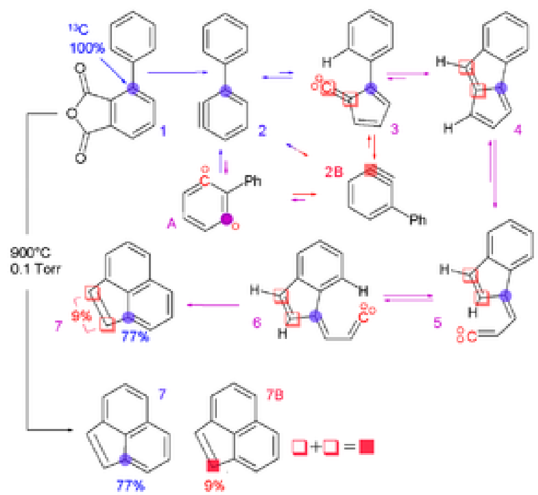
XPS of phosphorus

- Might see 1*s*, 2*s*, 2*p*

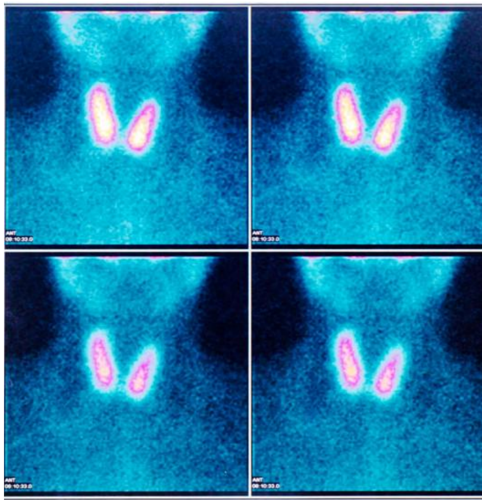


Why are isotopes significant?





https://en.wikipedia.org/wiki/File:Benzyneconversioncolouredlabels.png



https://www.healthline.com/health/thyroid-scan#uses

Unit 2: Molecular & Ionic Compounds

UNIT 2 Molecular and Ionic Compound Structure and Properties

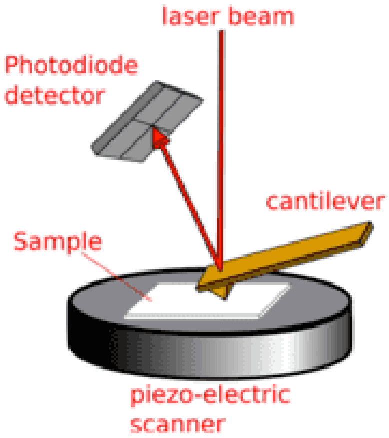
~12–13 Class Periods | 7–9% AP Exam Weighting

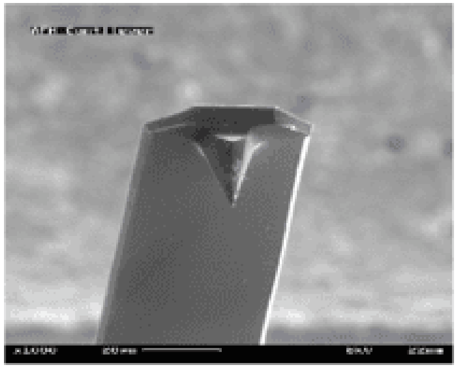
SAP 6	2.1	Types of Chemical Bonds
SAP 3	2.2	Intramolecular Force and Potential Energy
SAP 4	2.3	Structure of Ionic Solids
SAP 4	2.4	Structure of Metals and Alloys
SAP 3	2.5	Lewis Diagrams
SAP 6	2.6	Resonance and Formal Charge
SAP 6	2.7	VSEPR and Bond Hybridization

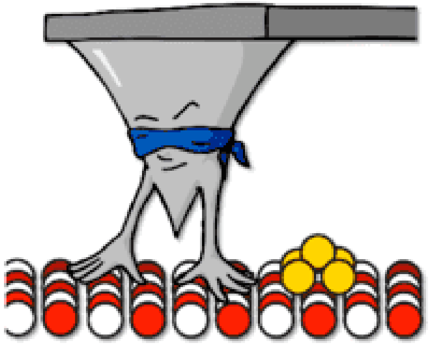
- Can we see bonds? Can we measure them?
- Effects of hybridization

Measuring Bond Length

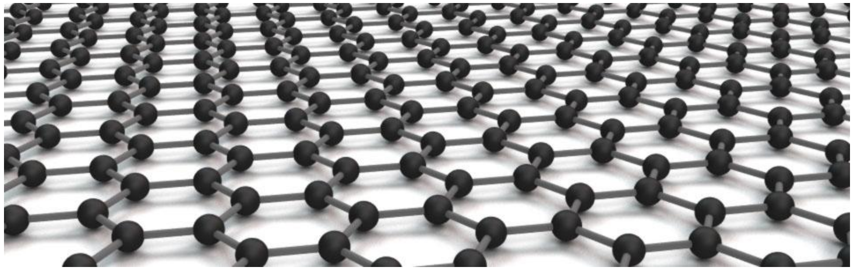
Atomic force microscopy (AFM)

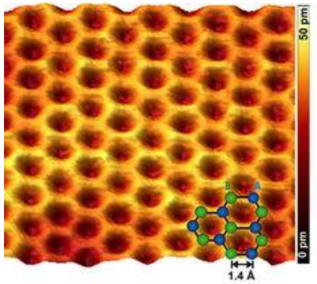






Graphene: a single layer of graphite





Sur, U. *Inter J of Electrochem*. (2012) 10.1155/2012/237689

Ionic vs. Covalent

Ionic "Bonding"

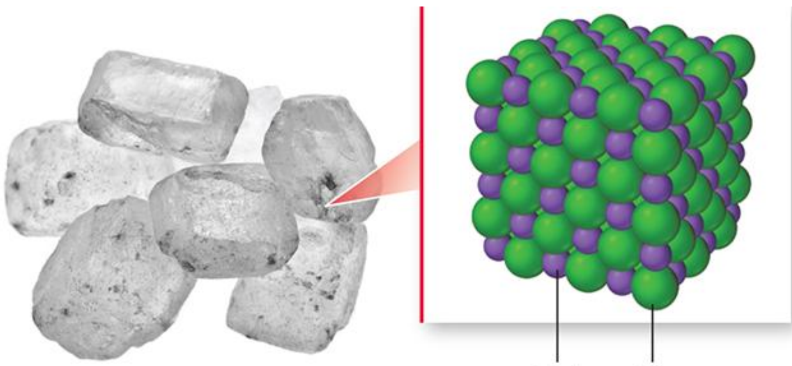
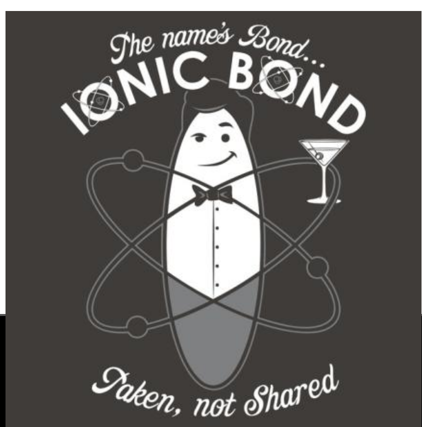
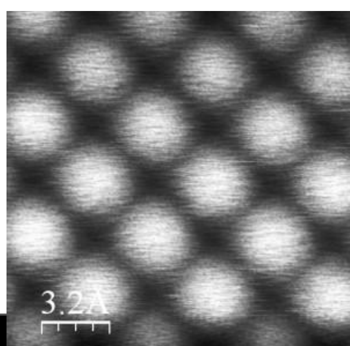
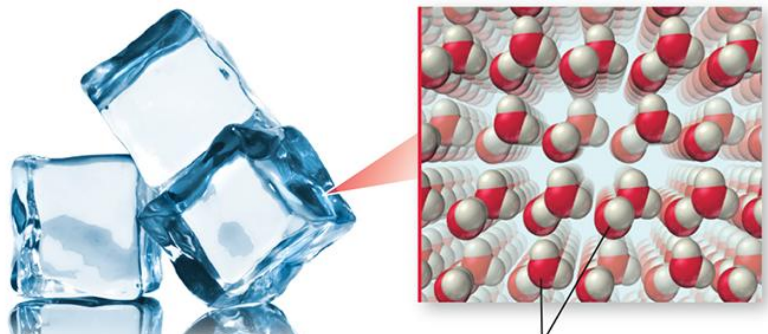


Table salt, NaCl(s)

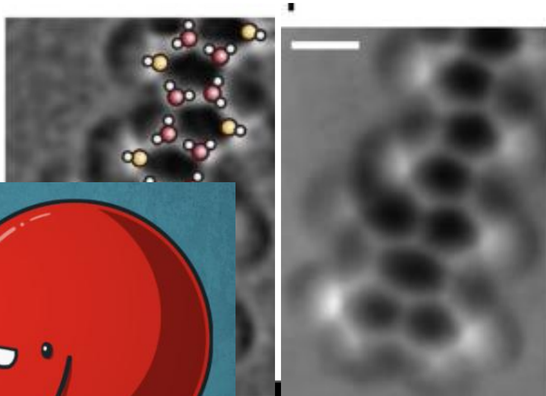


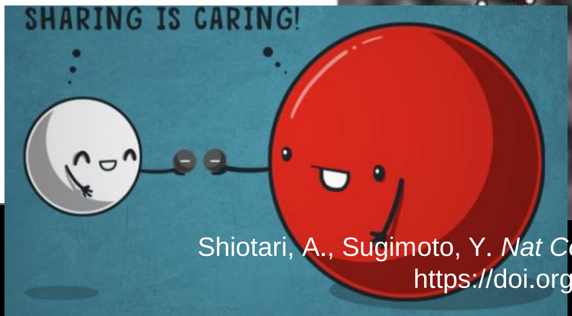


Covalent Bonding



Ice, $H_2O(s)$



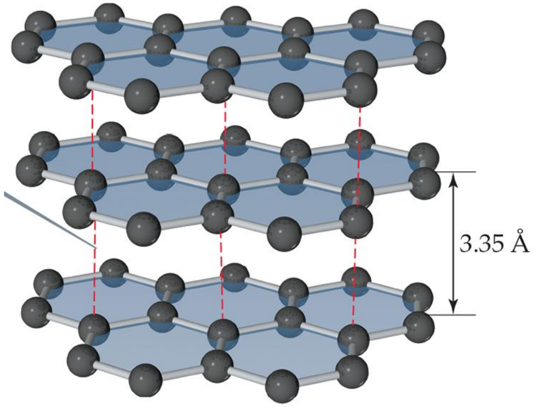


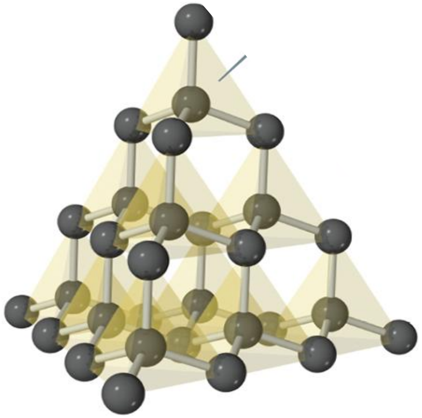
Shiotari, A., Sugimoto, Y. *Nat Commun* **8**, 14313 (2017). https://doi.org/10.1038/ncomms14313

What is the C hybridization?

Graphite (aka pencil lead)

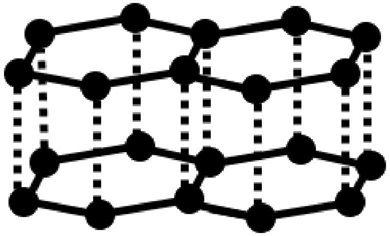
Diamond

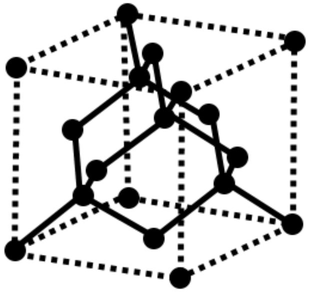




Graphite

Diamond





Unit 3: Intermolecular Forces

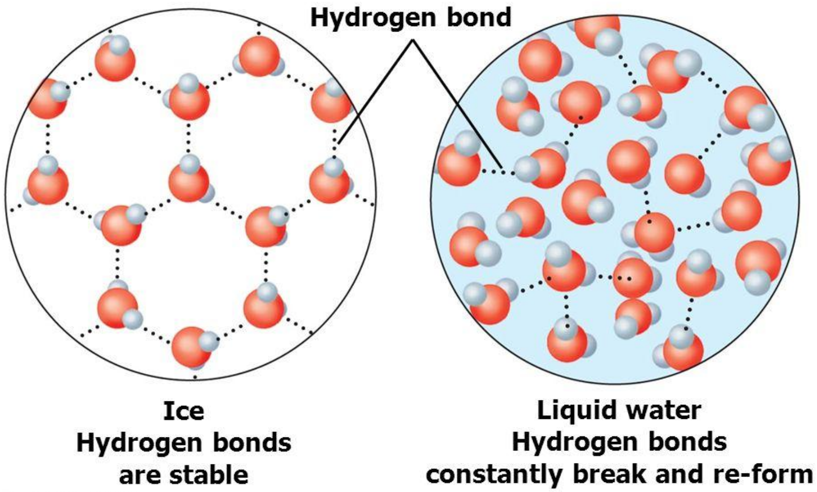
UNIT 3 Intermolecular Forces and Properties

~14–15 Class Periods | 18–22% AP Exam Weighting

- Shape of snowflakes
- Research: Non-Newtonain fluids
- Research: Janus particles
- Types of solids in everyday life

Snowflakes are shaped by IMFs!

Consider a single water molecule. How many water molecules can it hydrogen bond to (ignore crowding effects)?



A snowflake’s shape is determined by the interactions of hydrogen bonds during its formation.

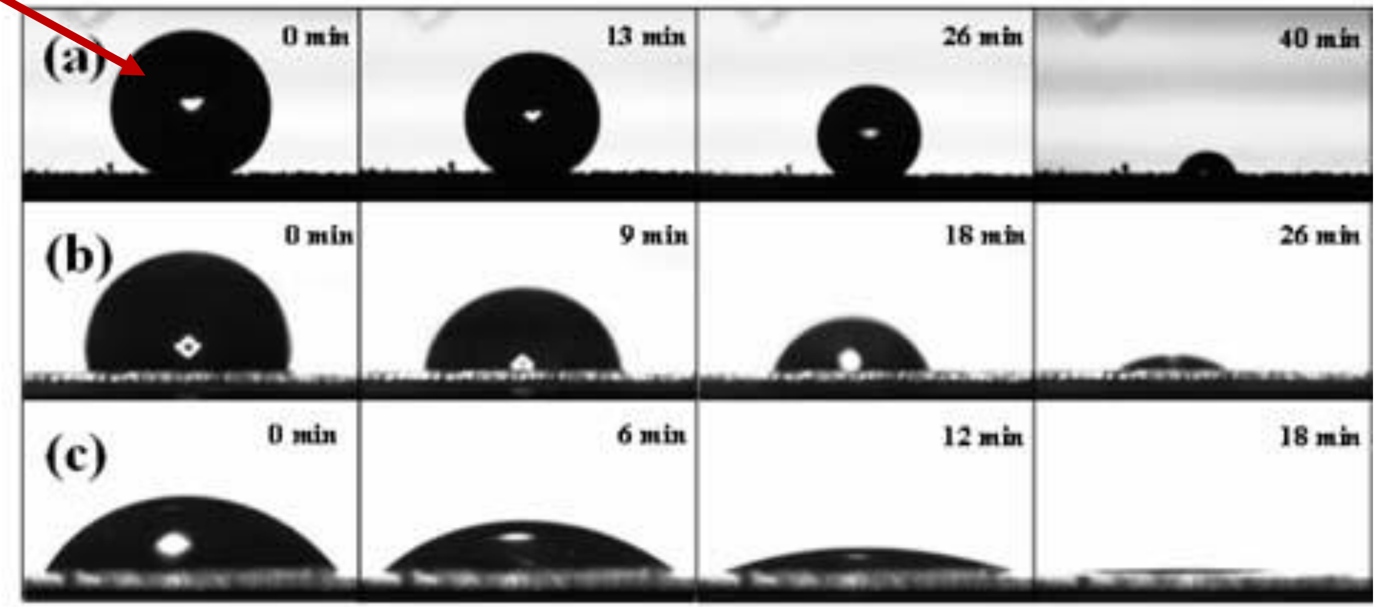
How does Gore-tex work?

Polar water

Super hydrophobic surface

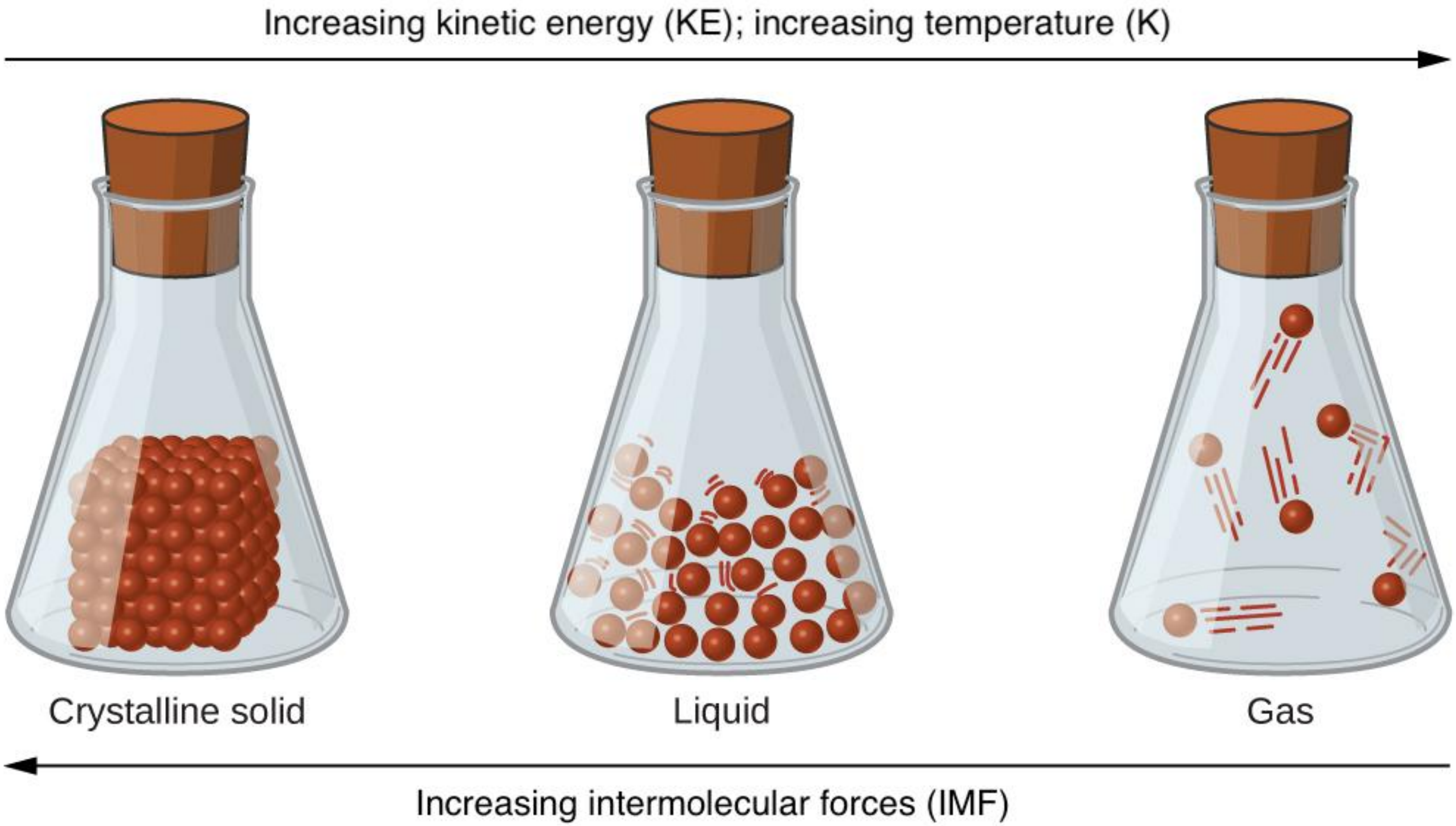
Hydrophobic surface

Hydrophilic surface



Choi, Chang K., “Evaporation characteristics of water droplets on super-hydrophobic surface.” (2022)

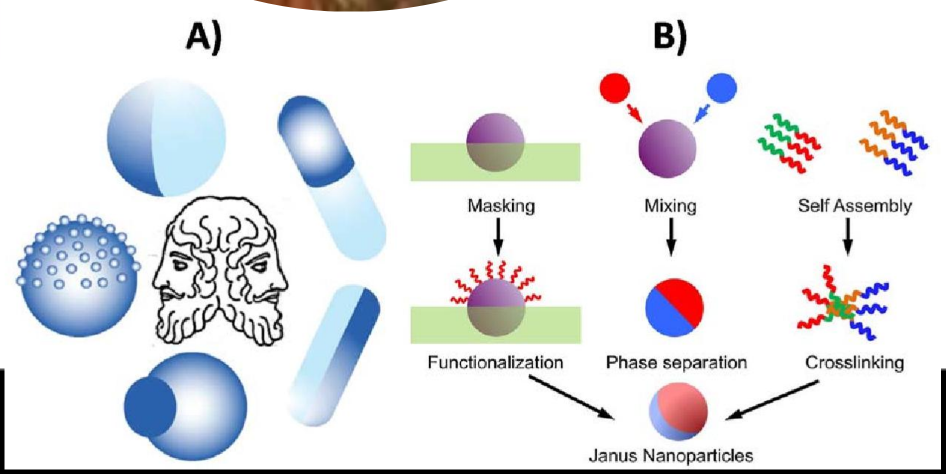
Non-Newtonian Fluids

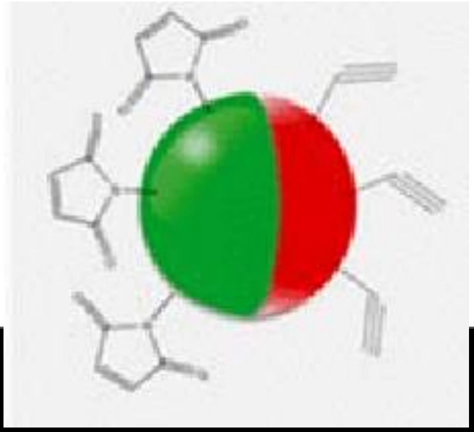


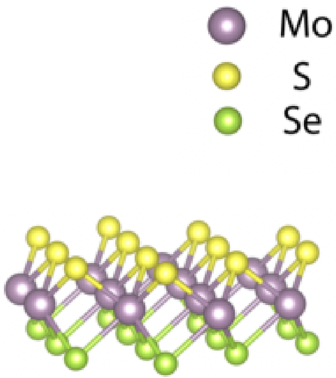
Fundamental difference: ***Distance between particles***

Janus Particles

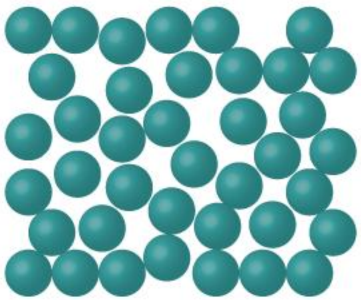
- Two-faced particles
  - Hydrophylic vs. hydrophobic
  - Self-assembly particles
  - Solar cells: n-type vs. p-type



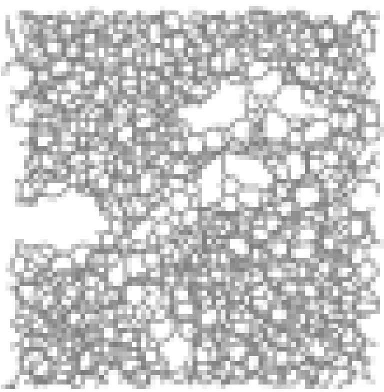




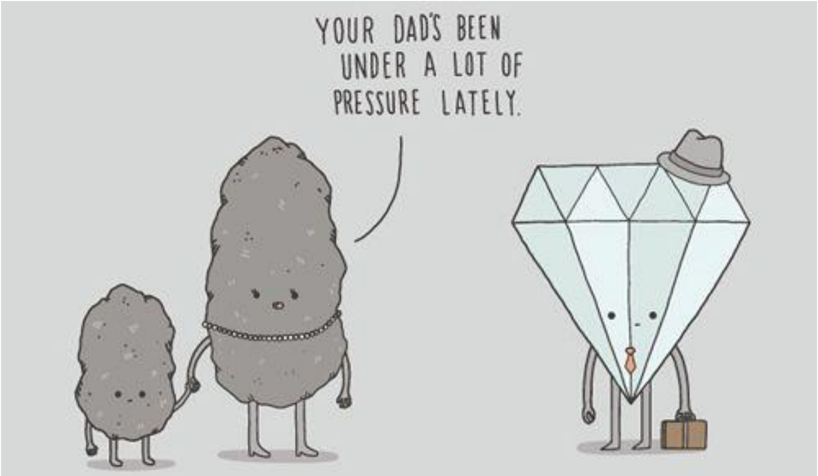
Amorphous vs. Crystalline Solids

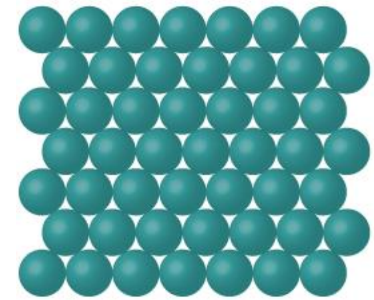


Amorphous

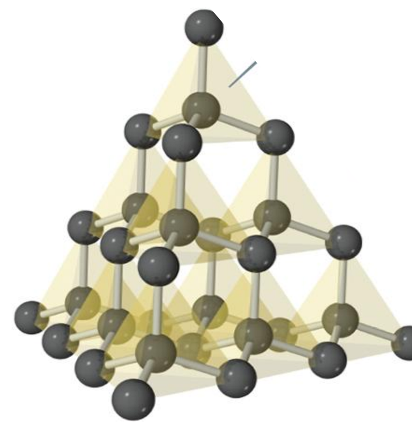


Charcoal





Crystalline



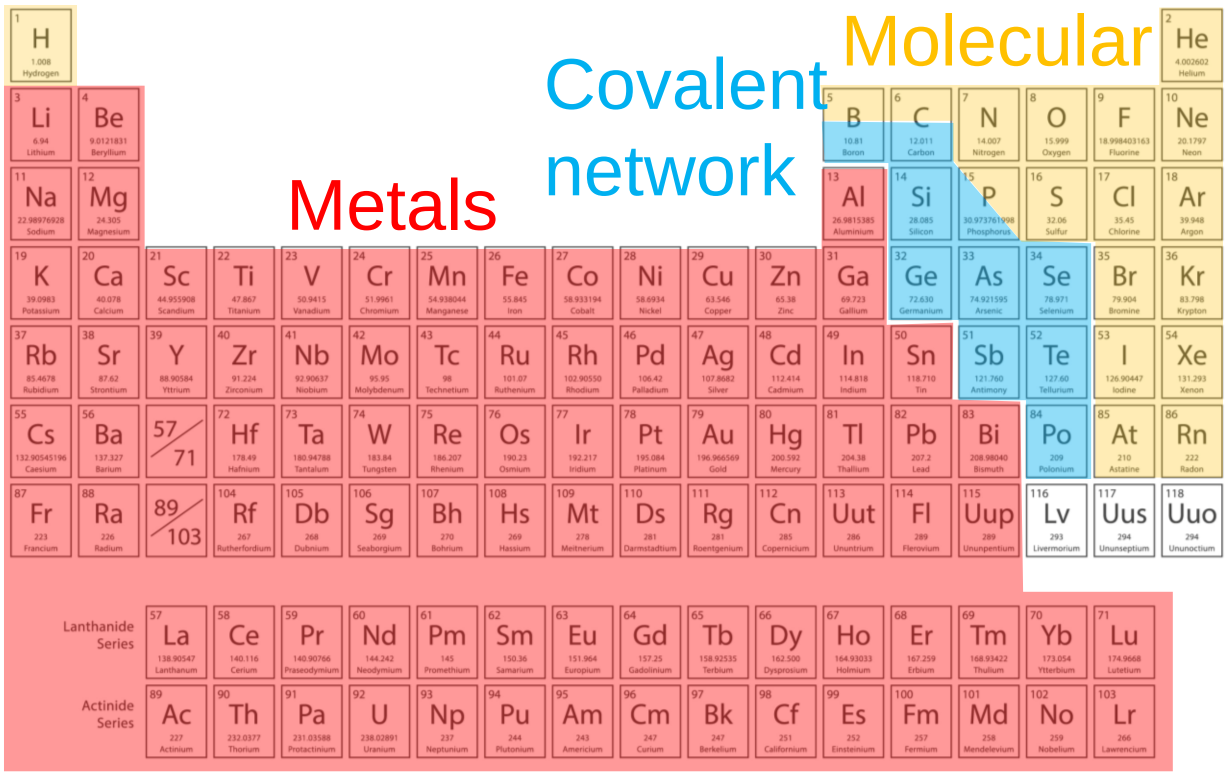
Diamond

Properties of Types of Crystalline Solids

Types of Crystalline Solids and Their Properties

Type of Solid	Type of Particles	Type of Attractions	Properties	Examples
ionic	ions	ionic bonds	hard, brittle, conducts electricity as a liquid but not as a solid, high to very high melting points	NaCl, Al_2O_3
metallic	atoms of electropositive elements	metallic bonds	shiny, malleable, ductile, conducts heat and electricity well, variable hardness and melting temperature	Cu, Fe, Ti, Pb, U
covalent network	atoms of electronegative elements	covalent bonds	very hard, not conductive, very high melting points	C (diamond), SiO_2, SiC
molecular	molecules (or atoms)	IMFs	variable hardness, variable brittleness, not conductive, low melting points	H_2O, CO_2, I_2, $C_{12}H_{22}O_{11}$

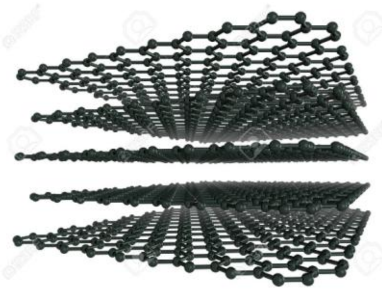
General Guide for Bonding in Solids

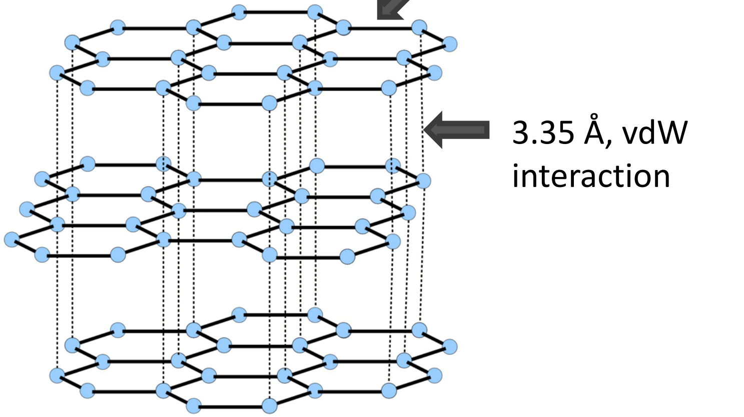


Ionic = metal + electronegative element

Graphite:

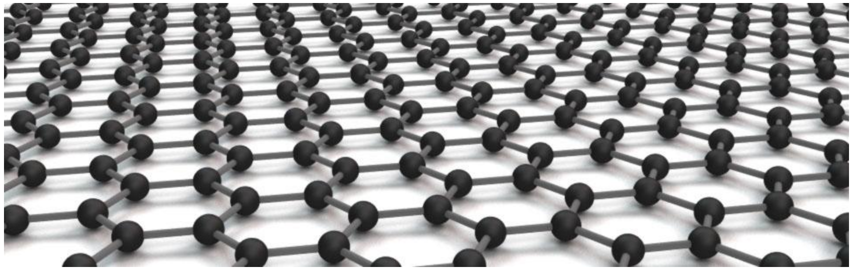
Graphite





Covalent-network (in plane) & Molecular (between planes)

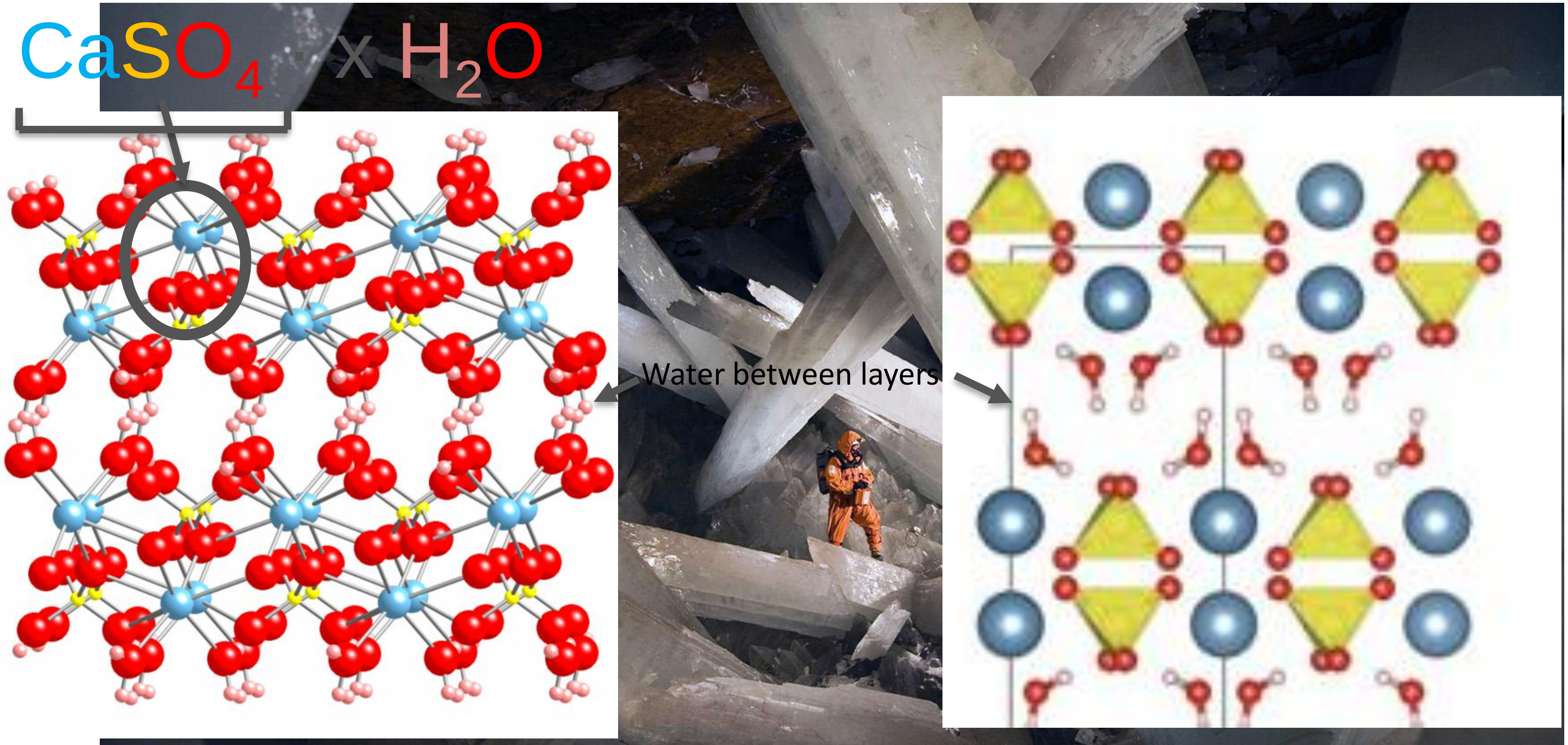
Graphene: a single layer of graphite



<u>Graphene is:</u>
The thinnest material
The strongest material (by weight)
The most conductive material
The most flexible material

Gypsum: Chalk, Plaster of Paris, Sheet Rock

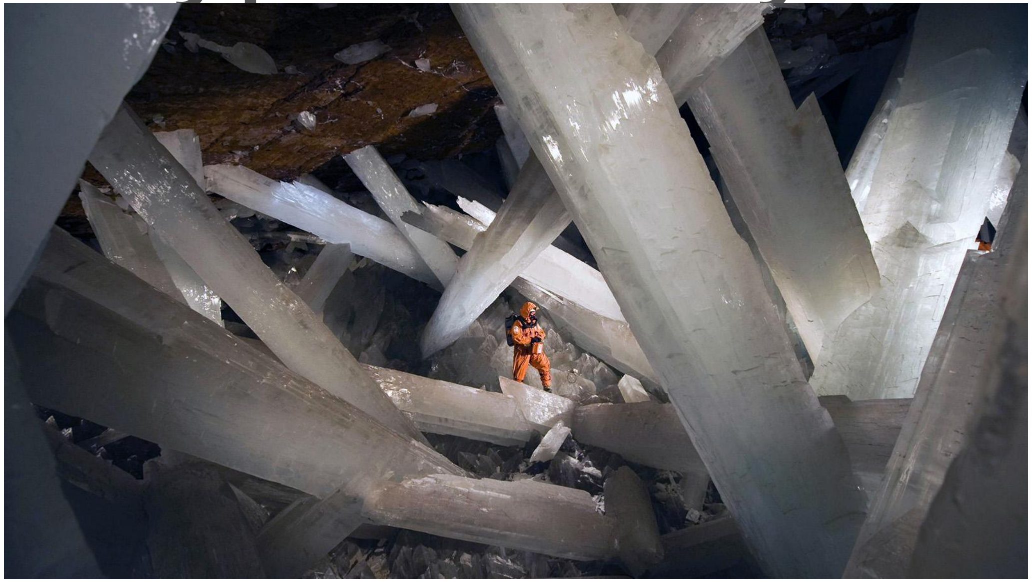
$CaSO_4 \cdot x\ H_2O$



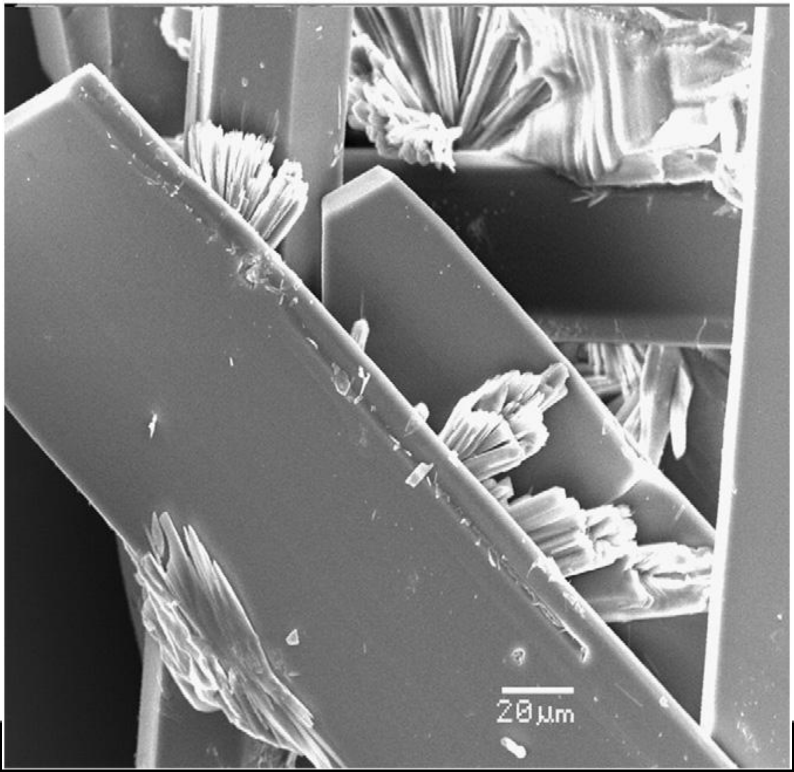
Ionic ($CaSO_4$ in-plane) & molecular (hydrogen bonding between planes)

A.E.S. Van Driessche et al. (eds.), New Perspectives on Mineral Nucleation and Growth, DOI 10.1007/978-3-319-45669-0_12

Gypsum: Crystals & SEM



Rahman, F. (2013). Calcium sulfate precipitation studies with scale inhibitors for reverse osmosis desalination. Desalination. 319. 79–84. 10.1016/j.desal.2013.03.027.



Unit 4: Chemical Reactions

UNIT 4 Chemical Reactions

~14–15 Class Periods | 7–9% AP Exam Weighting

TRA 2	4.1	Introduction for Reactions
TRA 5	4.2	Net Ionic Equations
TRA 3	4.3	Representations of Reactions
TRA 6	4.4	Physical and Chemical Changes
SPQ 5	4.5	Stoichiometry
SPQ 3	4.6	Introduction to Titration
TRA 1	4.7	Types of Chemical Reactions
TRA 1	4.8	Introduction to Acid-Base Reactions
TRA 5	4.9	Oxidation-Reduction (Redox) Reactions

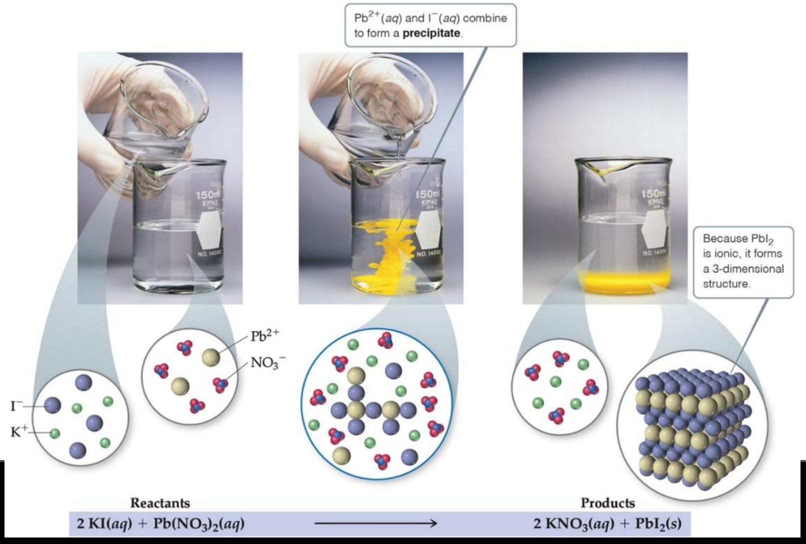
- Precipitating lead (very relevant in Utah)
- Combustion of Gasoline

Precipitation Reactions

Precipitation reactions occur when two solutions containing soluble salts are mixed and an insoluble salt is produced. The solid is called a **precipitate**.

For example: What happens when potassium iodide and lead (II) nitrate react? Be sure to include states of matter in the balanced chemical reaction.

$$2\,KI\,(aq) + Pb(NO_3)_2(aq) \rightarrow 2\,KNO_3(aq) + PbI_2(s)$$



D-Lead® Paint Test Kit from ESCA Tech, Inc

Lead-based paint was banned iin 1978 due to its toxic effects.

1. Lead in the paint is likely to have oxidized in air and formed lead (II) carbonate $PbCO_3$. A sample of paint is first placed in a basic solution (< 1 wt % NaOH).

$$PbCO_3\ (s) + 4\ OH^-\ (aq) \rightarrow Pb(OH)_4^{2-}\ (aq) + CO_3^{2-}\ (aq) \qquad K_1$$

2. Then, ammonium sulfide $(NH_4)_2S$ (< 2 wt%) is added to the previous mixture. If any lead cations are present, the following reaction will occur, producing brown lead (II) sulfide.

$$Pb(OH)_4^{2-}\ (aq) + (NH_4)_2S\ (aq) \rightarrow PbS\ (aq) + 2\ NH_4OH\ (aq) + 2\ OH^-\ (aq) \qquad K_2$$

Given that each of these reactions occur spontaneously at room temperature, what can be determined about the standard Gibbs Free Energy $\Delta G°$ for these processes (positive, negative, or zero)? (*2 pts*)

1) What can you determine about the equilibrium constant K_{eq} for these reactions ($K_{eq} > 1$, $K_{eq} < 1$, $K_{eq} = 1$)? Briefly support your answer. (*2 pts*)

-
-

D-Lead® Paint Test Kit from ESCA Tech, Inc

1. Given that each of these reactions occur spontaneously at room temperature, what can be determined about the standard Gibbs Free Energy $\Delta G°$ for these processes (positive, negative, or zero)?
2. What can you determine about the equilibrium constant K_{eq} for these reactions ($K_{eq} > 1$, $K_{eq} < 1$, $K_{eq} = 1$)? Briefly support your answer. Write the equilibrium constant K' for the net chemical reaction.
3. How is K' calculated based on K_1 and K_2?
4. The first reaction can only occur in basic conditions where the pH > 12. Calculate the pH of the < 1 wt% NaOH. Approximate the density of this solution as 1 g/mL at room temperature.
5. The detection limit of this reaction if 400 ppm Pb. What is the limiting reactant in this test: NaOH, $(NH_4)_2S$, or $PbCO_3$?

Combustion of Gasoline

Gasoline used in vehicles is a mixture of hydrocarbons that can be approximately represented by the formula C_8H_{18}. When this hydrocarbon combusts in an engine, it produces energy that can then be used to move a vehicle. Write the complete combustion reaction of gasoline in a car.

$$2C_8H_{18}(l) + 25O_2(g) \rightarrow 16CO_2(g) + 18H_2O(g)$$

Technology Highlights

- Oxidation
  - Ag vs. Al mirrors
  - Al_2O_3 vs CuO
- Selective adsorption
  - Scrubbing CO_2
- Surface functionalization
  - Sensors
- New material discovery & characterization

Unit 5: Kinetics

UNIT 5 Kinetics

~13–14 Class Periods | 7–9% AP Exam Weighting

TRA 6	5.1	Reaction Rates
TRA 5	5.2	Introduction to Rate Law
TRA 5	5.3	Concentration Changes Over Time
TRA 5	5.4	Elementary Reactions
TRA 6	5.5	Collision Model
TRA 3	5.6	Reaction Energy Profile
TRA 1	5.7	Introduction to Reaction Mechanisms
TRA 5	5.8	Reaction Mechanism and Rate Law
TRA 5	5.9	Steady-State Approximation
TRA 3	5.10	Multistep Reaction Energy Profile
ENE 6	5.11	Catalysis

- Lifetime of medicine
- Elephant toothpaste: Decomposition of H_2O_2
  - How yeast catalyzes this is still NOT KNOWN!

Kinetics & Pharmaceuticals

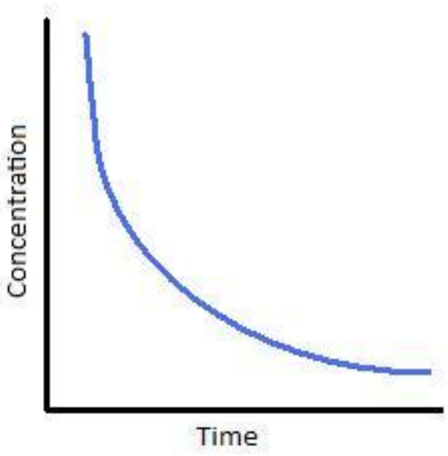
The chemotherapy drug Platinol is used to treat a variety of cancers. The change in concentration vs. time for Platinol is plotted below. Based on the graphs, is the hydrolysis of Platinol a zeroth, first, or second order reaction?

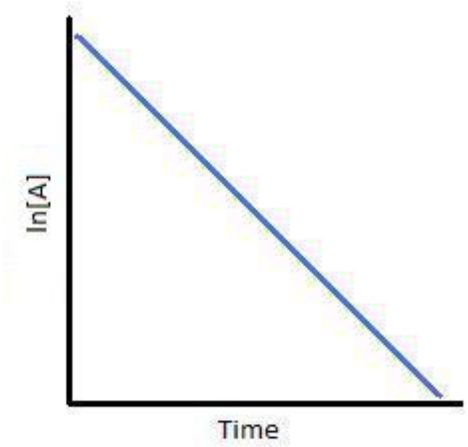
A. Zero

B. First

C. Second

D. Impossible to tell





Half-life & Pharmaceuticals

The rate constant for Platinol is 1.5×10^{-3} min^{-1} under physiological conditions. If the starting concentration of Platinol is 0.89 M, what is the half life of the drug?

A. 410 minutes

B. 440 minutes

C. 460 minutes

D. 520 minutes

$$\frac{0.693}{k} = t_{1/2}$$

Pro'cat' Kinetics

A cat has a daily dose of fluoxetine (Prozac) to treat her severe anxiety. When her owner goes out of town, the pet sitter is unable to get her to take her medicine. After missing five days of medicine, what percentage of the therapeutic level remains in the cat's blood? The half-life is 55 hours. Assume the drug is metabolized according to first-order kinetics.

Unit 6:Thermodynamics

UNIT 6 Thermodynamics

~10–11 Class Periods | 7–9% AP Exam Weighting

- ENE 6 — 6.1 Endothermic and Exothermic Processes
- ENE 3 — 6.2 Energy Diagrams
- ENE 6 — 6.3 Heat Transfer and Thermal Equilibrium
- ENE 2 — 6.4 Heat Capacity and Calorimetry
- ENE 1 — 6.5 Energy of Phase Changes
- ENE 4 — 6.6 Introduction to Enthalpy of Reaction
- ENE 5 — 6.7 Bond Enthalpies
- ENE 5 — 6.8 Enthalpy of Formation
- ENE 5 — 6.9 Hess's Law

- “Kitchen chemistry”
- Phase Changes of NaCl
- Supercritical fluids
- Research: Supercooled fluiids
- Research: Solid Phase
- Research: 2D solids
- Calorimetry

Instapot: Chemistry or Hoax?

The Instapot™ is an electric pressure cooker that claims to reduce the time necessary to prepare foods. How does it work?

A. The Instapot™ decreases the pressure in the cooker, thus decreasing the boiling point (BP) of water. As the water is heated, it boils more quickly and so cooks the food more quickly.

B. The Instapot™ increases the pressure in the cooker, thus increasing the BP of water, and the food is cooked more quickly because it is cooking at a higher temperature.

C. The Instapot™ increases the pressure in the cooker, thus decreasing the BP of water, and the food is cooked more quickly because it reaches the BP more quickly.

D. Although the Instapot™ changes the pressure inside the cooker, it only affects the vapor pressure, not the BP, of water. Food is cooked faster because all the heat is kept in the cooker.

E. The Instapot is a gimmick.

High Altitude Recipes: WHY?

Many recipes have different instructions for baking at higher altitudes, including using a higher temperature. This is due to the differences in atmospheric pressure and its effect on cooking conditions.

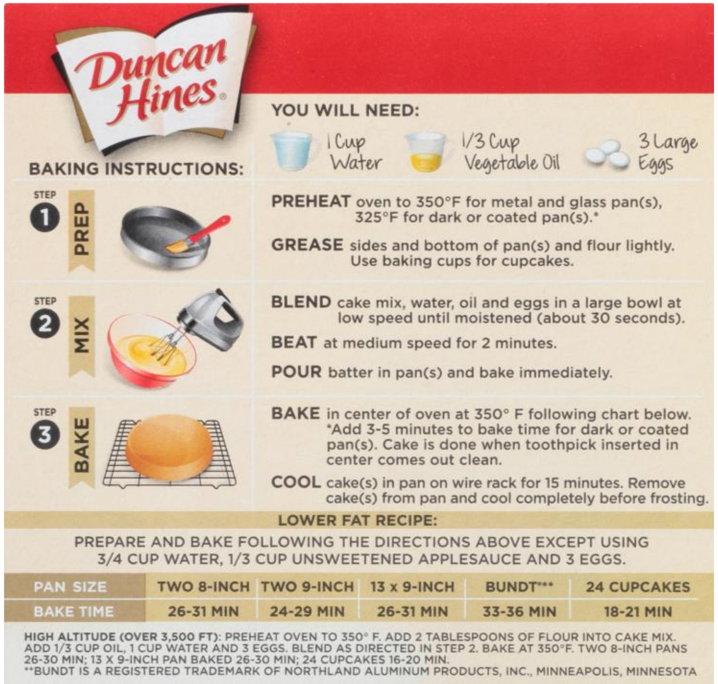
At a higher altitude, atmospheric pressure is _____, therefore water boils at a _____ temperature.

A. < 1 atm, higher

B. < 1 atm, lower

C. > 1 atm, higher

D. > 1 atm, lower



R = 8.314 J K^{-1} mol^{-1}

Boiling Point of NaCl

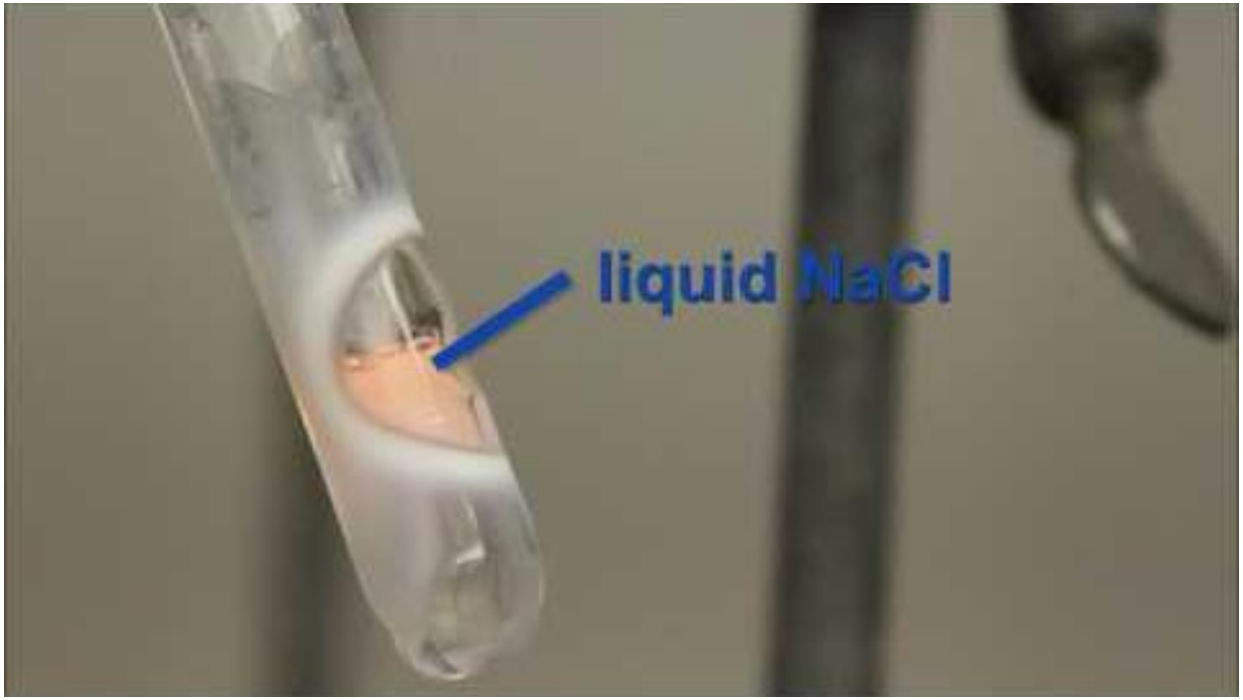
Sodium chloride melts at 801 ^oC. Molten NaCl has a vapor pressure of 6.12 torr at 977^oC and 8.66 torr at 1003 ^oC.

What is its normal boiling point?

$$\ln\left(\frac{p_2}{p_1}\right) = \frac{\Delta H_{vap}}{R}\left[\frac{1}{T_1} - \frac{1}{T_2}\right]$$

Can you really boil NaCl?

Courtesy of Dr. Scott Warren, UNC Department of Chemistry



Supercritical Fluids

Behave like a liquid & gas:

- the fluid fills a container completely (like a gas)
- the fluid is much denser than a gas (like a liquid).

Supercritical fluids are produced when:

1. Temperatures are high enough to overcome intermolecular forces.
2. Pressures are high enough to achieve high densities.

Supercritical CO_2

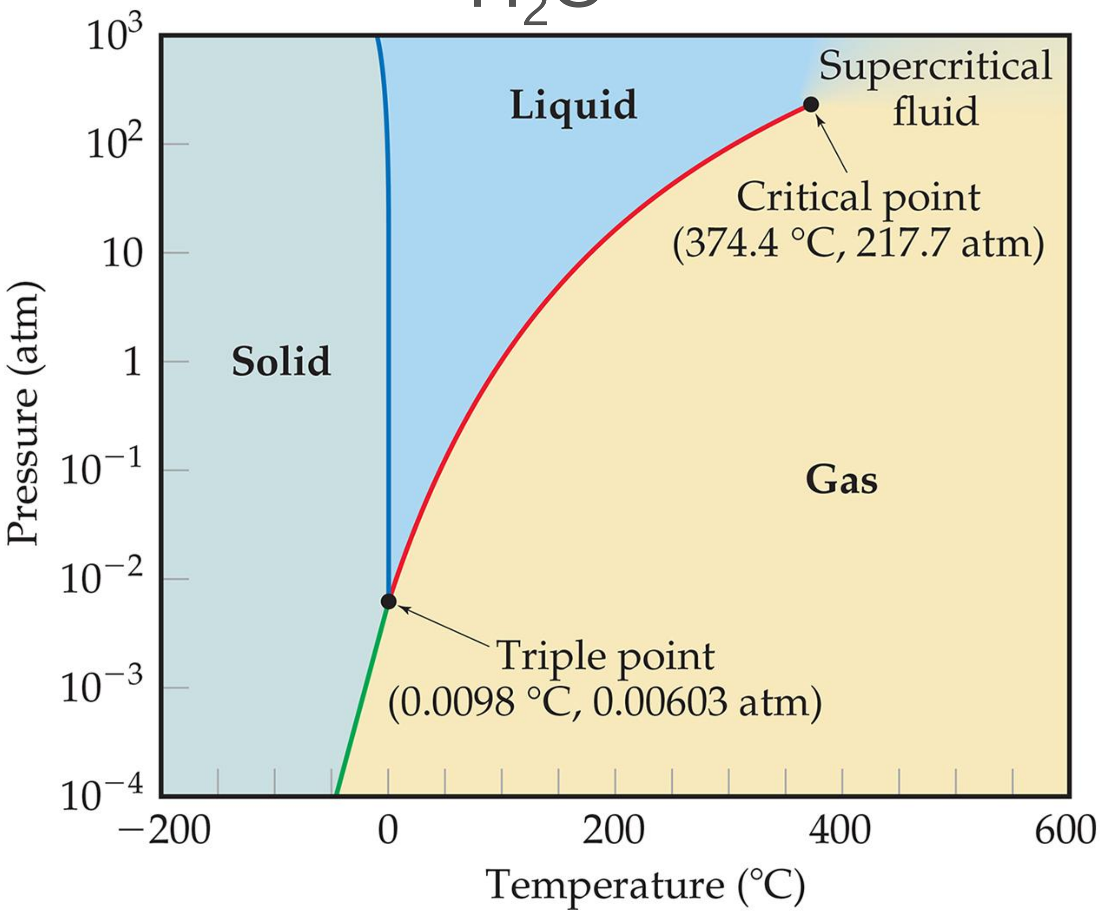
1. Non-polar.
   - Dissolves non-polar substances. (“Like dissolves like.”)
2. Enters materials like a gas.
3. Tunable density.
4. Cannot be oxidized.
5. Volatile.
6. Non-toxic.

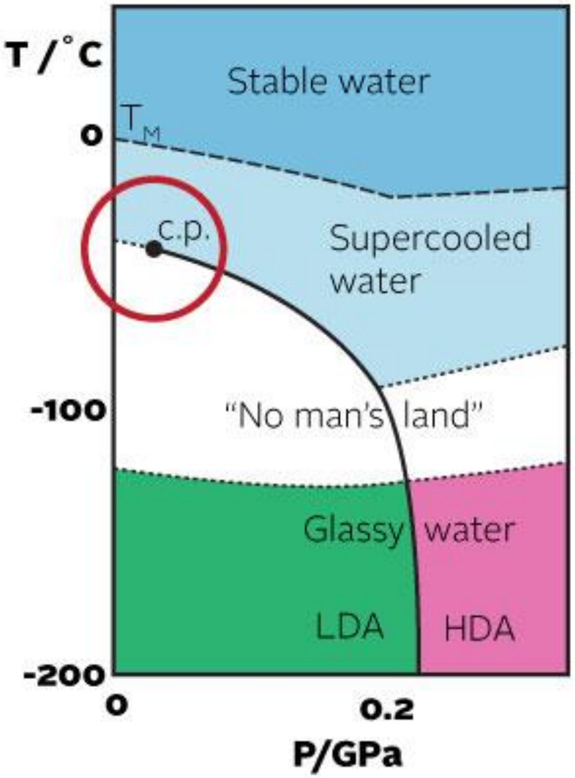
Supercritical fluids has replaced toxic solvents in certain applications, including:

- a solvent for dry cleaning
- a solvent for extracting caffeine from coffee beans

Research: Supercooled fluids

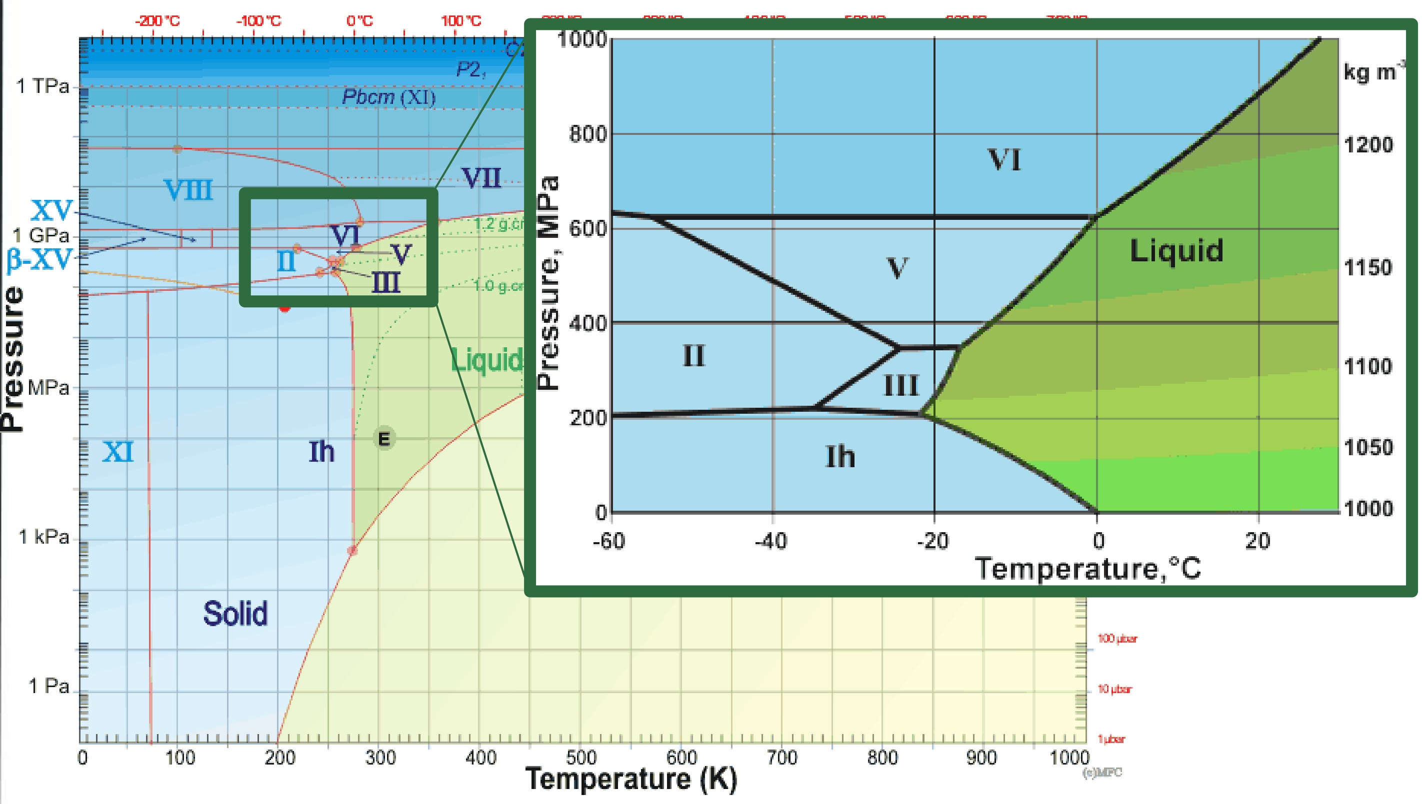
H_2O





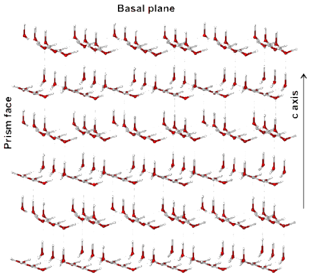
Wynne Lab, University of Glasgow

Research: Different Solid Phases

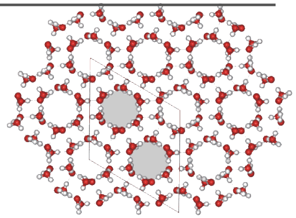


Link to different phases here

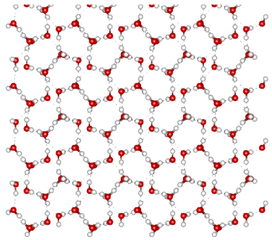
Ih – Hexagonal



II - Rhombohedral

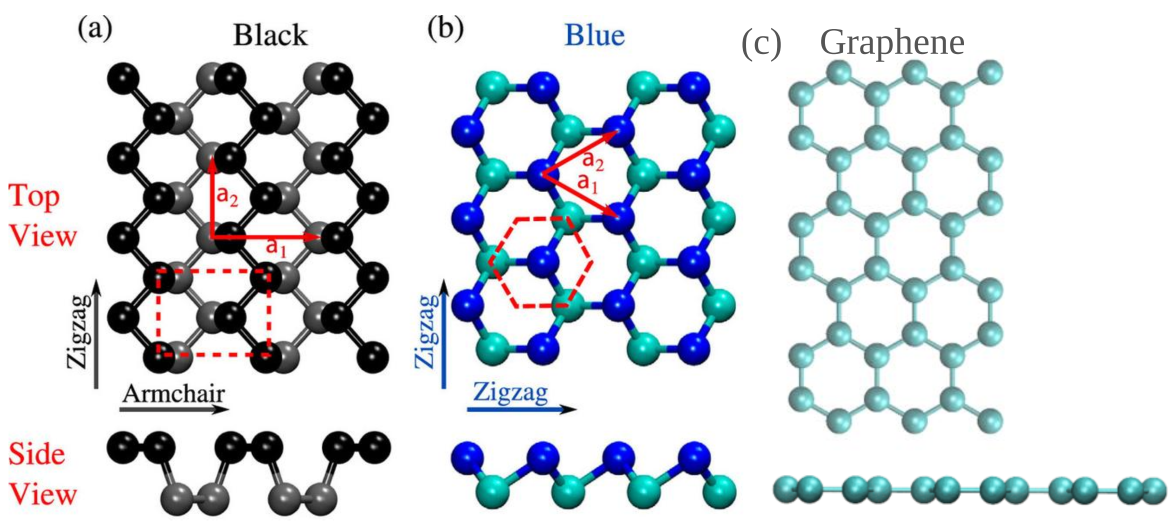


III - Tetragonal



Research: 2D Solids

- Black Phosphorus: direct gap semiconductor, sp^3
- Blue phosphorene: indirect semiconductor, sp^2 hybridization
- Graphene: semimetal, sp^2 hybridization, honeycomb



Jain, Ankit & Mcgaughey, Alan. (2015). Strongly anisotropic in-plane thermal transport in single-layer black phosphorene. Scientific reports. 5. 8501. 10.1038/srep08501.

Where do we use calorimetry and enthalpy?

Food

Vitamin D Milk

Nutrition Facts
Serving Size 1 cup (236mL)

Amount Per Serving	
Calories 150	Calories from Fat 70
	% Daily Value*
Total Fat 8g	**12%**
Saturated Fat 5g	**25%**
Trans Fat 0g	
Cholesterol 35mg	**11%**
Sodium 125mg	**5%**
Total Carbohydrate 12g	**4%**
Dietary Fiber 0g	**0%**
Sugars 12g	
Protein 8g	

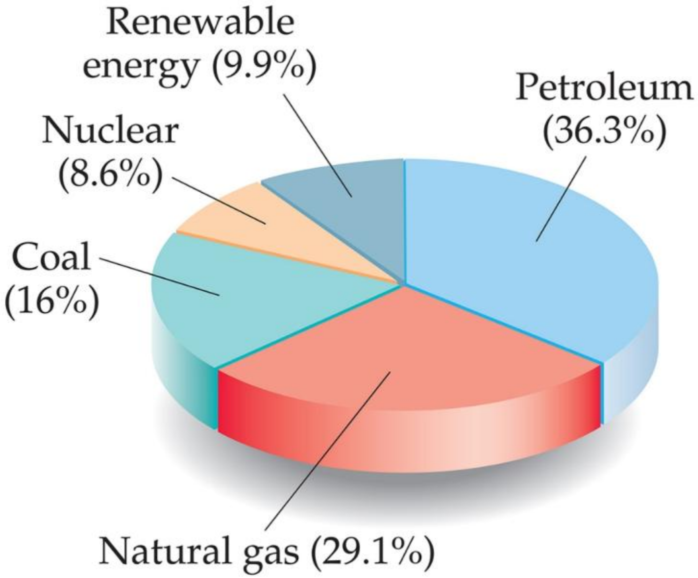
Vitamin A 6% • Vitamin C 4%
Calcium 30% • Iron 0%
Vitamin D 25%

* Percent Daily Values are based on a 2,000 calorie diet. Your daily values may be higher or lower depending on your calorie needs.

		Calories: 2,000	2,500
Total fat	Less than	65g	80g
Sat Fat	Less than	20g	25g
Cholesterol	Less than	300mg	300mg
Sodium	Less than	2,400g	2,400g
Total Carbohydrate		300g	375g
Dietary Fiber		25g	30g

Ingredients: Grade A Pasteurized Milk, Vitamin D3.

Fuel



Unit 7: Equilibrium

UNIT 7 Equilibrium

~14–16 Class Periods | 7–9% AP Exam Weighting

- TRA 6 — 7.1 Introduction to Equilibrium
- TRA 4 — 7.2 Direction of Reversible Reactions
- TRA 3 — 7.3 Reaction Quotient and Equilibrium Constant
- TRA 5 — 7.4 Calculating the Equilibrium Constant
- TRA 6 — 7.5 Magnitude of the Equilibrium Constant
- TRA 5 — 7.6 Properties of the Equilibrium Constant
- TRA 3 — 7.7 Calculating Equilibrium Concentrations
- TRA 3 — 7.8 Representations of Equilibrium
- TRA 6 — 7.9 Introduction to Le Châtelier's Principle
- TRA 5 — 7.10 Reaction Quotient and Le Châtelier's Principle
- SPQ 5 — 7.11 Introduction to Solubility Equilibria
- SPQ 2 — 7.12 Common-Ion Effect
- SPQ 2 — 7.13 pH and Solubility
- SPQ 4 — 7.14 Free Energy of Dissolution

- Haber process
- Ocean acidification
- Mining Quarries & Basicity
- Every day life: Ammonia

Research: Haber Process

Haber Process

$$3H_2(g) + N_2(g) \rightleftharpoons 2NH_3(g)$$

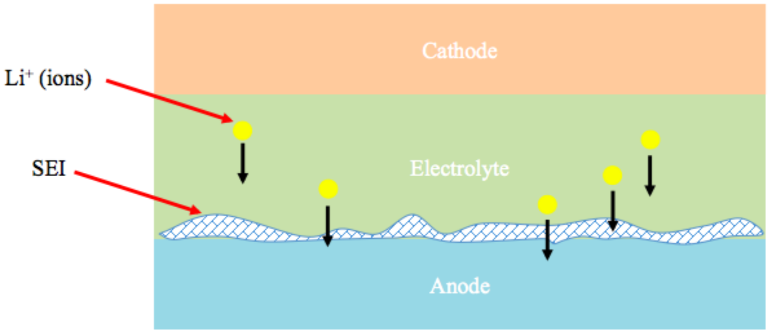
Exothermic: $\Delta H < 0$ $K_{eq} = 6.8 \times 10^5$

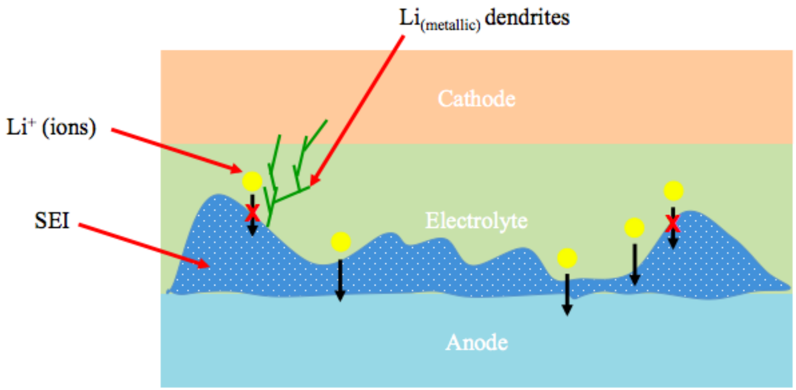
- We have not achieved a production yield of ammonia above 15%.
  - However, if we could improve the yield of ammonia, we could produce sufficient fertilizer to adequately address food needs around the world.

https://areweanycloser.wordpress.com/2013/06/21/dendritic-lithium-and-battery-fires/

Research: Li-Ion Batteries

- Li-ion Batteries





https://areweanycloser.wordpress.com/2013/06/21/dendritic-lithium-and-battery-fires/

Homework Question

In old mining sites, such as this rock quarry, water can collect. Over time, minerals become dissolved in the water and alter its pH.

If $CaNO_3$ dissolves into the water, what would the pH be?

Question

For this aqueous reaction in household ammonia

$$NH_3 + H_2O \rightleftharpoons NH_4^+ + OH^-$$

$K_b = 1.8 \cdot 10^{-5}$ at 25°C. At equilibrium, _____.

A. products dominate the system mixture.

B. reactants dominate the system mixture.

C. roughly equal amounts of products and reactants are present in the system mixture.

D. only products are present.

E. only reactants are present.

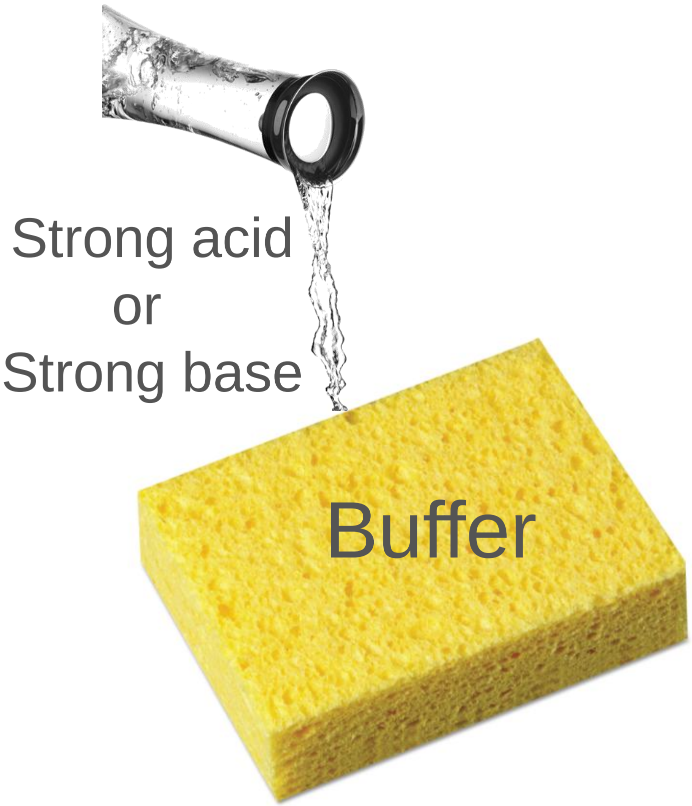
Unit 8: Acids and Bases

UNIT 8 Acids and Bases

~14–15 Class Periods | 11–15% AP Exam Weighting

- Making Cheese/Tofu/etc
- Human Buffers

What is a buffer?



Buffers soak up H^+ from a strong acid or the OH^- from a strong base.

What is a buffer? Buffers are mixtures that resist changes in pH.

If you add strong acid or strong base to a buffer, the pH won't change much.

Our bodies function because our blood is a buffer with a pH of 7.45.

Buffers in the body

The equilibrium system that buffers blood is:

$$H_2CO_3(aq) + H_2O(l) \rightleftharpoons HCO_3^-(aq) + H_3O^+(aq)$$

What is the ratio of [HCO_3^-] to [H_2CO_3] in blood at pH 7.45?

$K_a(H_2CO_3) = 4.3 \times 10^{-7}$

Unit 9: Applications of Thermodynamics

UNIT 9 Applications of Thermodynamics

~10–13 Class Periods | 7–9% AP Exam Weighting

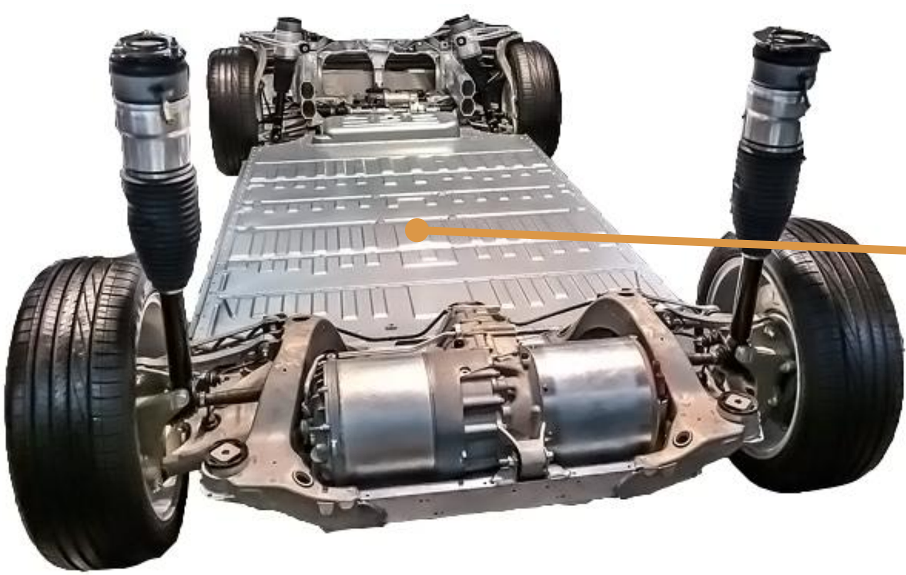
ENE 6	9.1	Introduction to Entropy
ENE 5	9.2	Absolute Entropy and Entropy Change
ENE 6	9.3	Gibbs Free Energy and Thermodynamic Favorability
ENE 6	9.4	Thermodynamic and Kinetic Control
ENE 6	9.5	Free Energy and Equilibrium
ENE 4	9.6	Coupled Reactions
ENE 2	9.7	Galvanic (Voltaic) and Electrolytic Cells
ENE 5	9.8	Cell Potential and Free Energy
ENE 6	9.9	Cell Potential Under Nonstandard Conditions
ENE 5	9.10	Electrolysis and Faraday's Law

- Batteries
  - Primary Batteries (1971)
    - e.g. Car batteries
  - Secondary Batteries (recharge)
    - e.g. Li-ion

Galvanic Cells (or Voltaic Cells)

Galvanic cells have:

- oxidation-reduction reactions
  - electrical energy can be utilized
- the reactions occur spontaneously
  - ΔG is negative (ΔE is positive)



Floor of Tesla Model S
500 kg (1000 pounds) of batteries

Car Batteries: 12 V

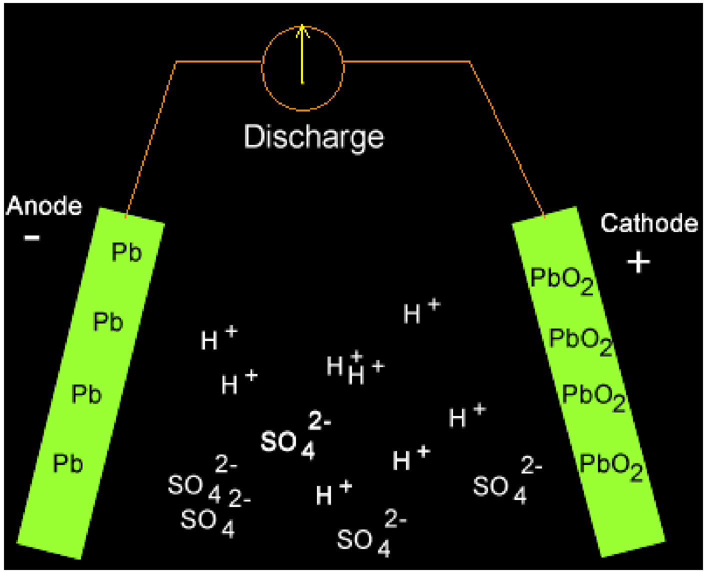
- 6 Galvanic Cells in series
  - Approximate voltage from each

$$E^{o}_{cell} = E^{o}_{red}(cathode) - E^{o}_{red}(anode)$$

Calculate the voltage produced by each cell.

Car Batteries: 12 V

- 6 Galvanic Cells in series
  - Approximate voltage from each cell:



$$E^o_{cell} = E^o_{red}(cathode) - E^o_{red}(anode)$$

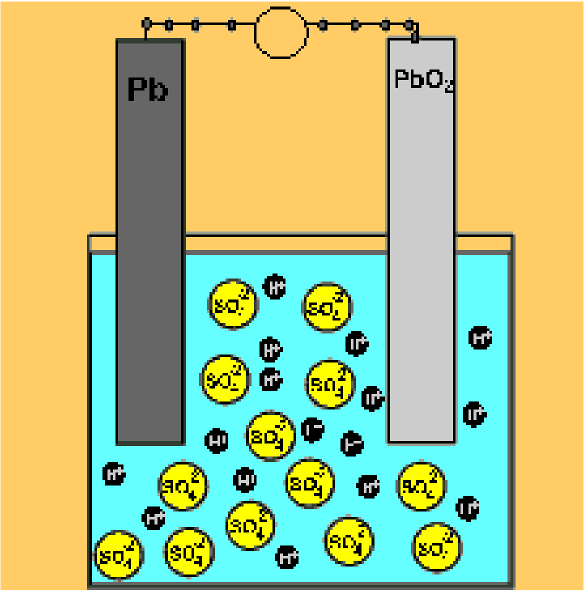
Calculate the voltage produced by each cell.

$PbO_2(s) + H_2SO_4(aq) + 2H^+(aq) + 2\,e^- \rightarrow 2\,PbSO_4(s) + 2H_2O(l)$ $E^\circ_{red} = +1.69\,V$

$PbSO_4(s) + 2\,H^+(aq) + 2\,e^- \rightarrow Pb(s) + H_2SO_4(aq)$ $E^\circ_{red} = -0.35\,V$

$PbO_2(s) + Pb(s) + 2H_2SO_4(aq) \rightarrow 2\,PbSO_4(s) + 2\,H_2O(l)$ $E^\circ_{cell} = +2.04\,V$

Car Battery: 12 V



$$PbO_2(s) + H_2SO_4(aq) + 2H^+(aq) + 2\,e^- \rightarrow 2\,PbSO_4(s) + 2H_2O(l) \qquad E^\circ_{red} = +1.69\,V$$

$$PbSO_4(s) + 2\,H^+(aq) + 2\,e^- \rightarrow Pb(s) + H_2SO_4(aq) \qquad E^\circ_{red} = -0.35\,V$$

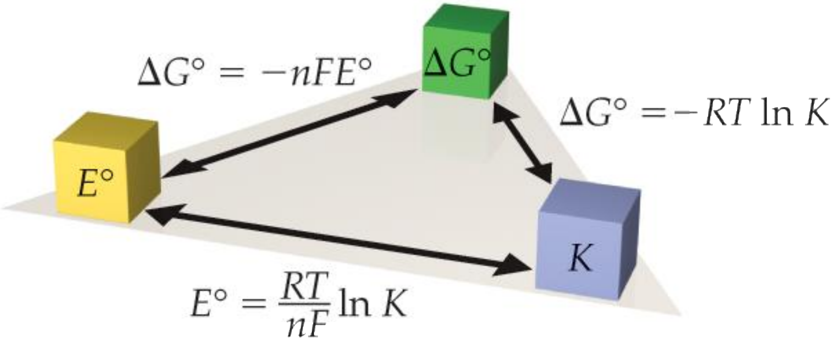
$$PbO_2(s) + Pb(s) + 2H_2SO_4(aq) \rightarrow 2\,PbSO_4(s) + 2\,H_2O(l) \qquad E^\circ_{cell} = +2.04\,V$$

Car Batteries: Gibbs Free Energy

Calculate the standard Gibbs free energy $\Delta G°$ for the car battery.

$$PbO_2(s) + H_2SO_4(aq) + 2H^+(aq) + 2\,e^- \rightarrow 2\,PbSO_4(s) + 2H_2O(l) \quad E°_{red} = +1.69\,V$$
$$PbSO_4(s) + 2\,H^+(aq) + 2\,e^- \rightarrow Pb(s) + H_2SO_4(aq) \quad E°_{red} = -0.35\,V$$

$$PbO_2(s) + Pb(s) + 2H_2SO_4(aq) \rightarrow 2\,PbSO_4(s) + 2\,H_2O(l) \quad E°_{cell} = +2.04\,V$$



1 F = 96,485 C/mol = 96,485 J/V-mol

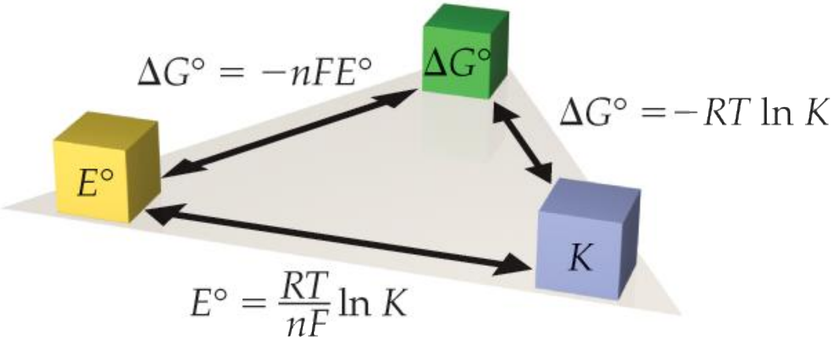
Car Batteries: Equilibrium Constant

Calculate the equilibrium constant K for the car battery at $25°C$.

$$PbO_2(s) + H_2SO_4(aq) + 2H^+(aq) + 2\,e^- \rightarrow 2\,PbSO_4(s) + 2H_2O(l) \qquad E^\circ_{red} = +1.69\,V$$

$$PbSO_4(s) + 2\,H^+(aq) + 2\,e^- \rightarrow Pb(s) + H_2SO_4(aq) \qquad E^\circ_{red} = -0.35\,V$$

$$PbO_2(s) + Pb(s) + 2H_2SO_4(aq) \rightarrow 2\,PbSO_4(s) + 2\,H_2O(l) \qquad E^\circ_{cell} = +2.04\,V$$

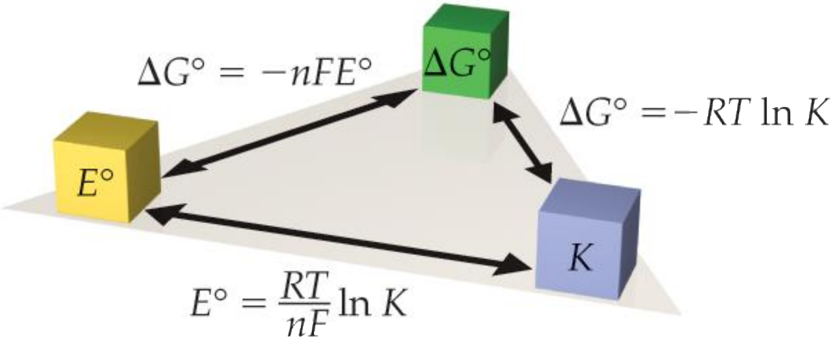


1 F = 96,485 C/mol = 96,485 J/V-mol

When do batteries work best?

What happens to E_{cell} as temperature increases? Explain.

Often times, people store their batteries in the fridge. Is this a good or bad practice? Explain.



Car Batteries: Non-standard Conditions

What would happen to the value of K if the battery acid were less concentrated?

What would happen to the voltage produced?

$$PbO_2(s) + H_2SO_4(aq) + 2H^+(aq) + 2\,e^- \rightarrow 2\,PbSO_4(s) + 2H_2O(l) \qquad E^\circ_{red} = +1.69\,V$$

$$PbSO_4(s) + 2\,H^+(aq) + 2\,e^- \rightarrow Pb(s) + H_2SO_4(aq) \qquad E^\circ_{red} = -0.35\,V$$

$$PbO_2(s) + Pb(s) + 2H_2SO_4(aq) \rightarrow 2\,PbSO_4(s) + 2\,H_2O(l) \qquad E^\circ_{cell} = +2.04\,V$$

Nernst Equation

Recall, $\Delta G = \Delta G^o + RT\ln Q$ and $\Delta G = -nFE$

So,

$$-nFE = -nFE^o + RT\ln Q$$

By dividing by *-nF*, we get

$$\mathrm{E} = \mathrm{E^o} - \frac{\mathrm{RT}}{\mathrm{nF}}\ln \mathrm{Q}$$

At room temperature and converting ln to log, we get

$$\mathrm{E} = \mathrm{E^o} - \frac{0.05916}{\mathrm{n}}\log \mathrm{Q}$$

Car Batteries: Non-standard Conditions

Calculate the voltage produced if the concentrations are changed and the reaction quotient Q = 1 x 10^3 on a hot summer day at 38^oC.

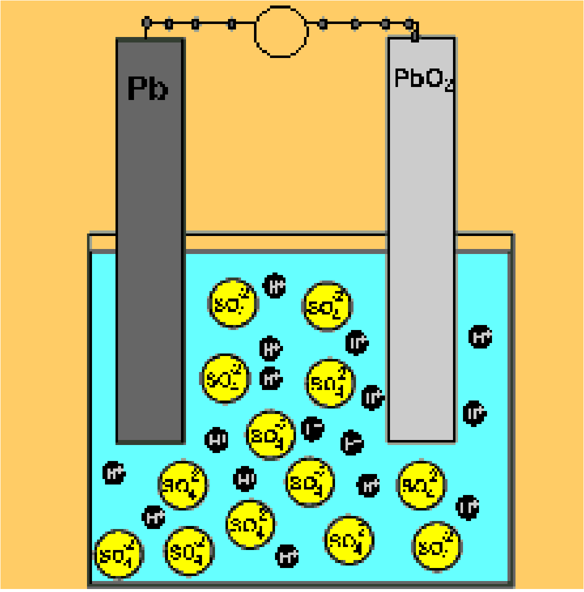
$$E = E^o - \frac{RT}{nF} \ln Q$$

$$PbO_2(s) + H_2SO_4(aq) + 2H^+(aq) + 2\,e^- \rightarrow 2\,PbSO_4(s) + 2H_2O(l) \qquad E^\circ_{red} = +1.69\,V$$

$$PbSO_4(s) + 2\,H^+(aq) + 2\,e^- \rightarrow Pb(s) + H_2SO_4(aq) \qquad E^\circ_{red} = -0.35\,V$$

$$PbO_2(s) + Pb(s) + 2H_2SO_4(aq) \rightarrow 2\,PbSO_4(s) + 2\,H_2O(l) \qquad E^\circ_{cell} = +2.04\,V$$

How to shrink down to small battery?



Same solution at the cathode, anode, and for salt bridge!

This solution *must* conduct electricity and *must* allow molecules to diffuse (move) easily.

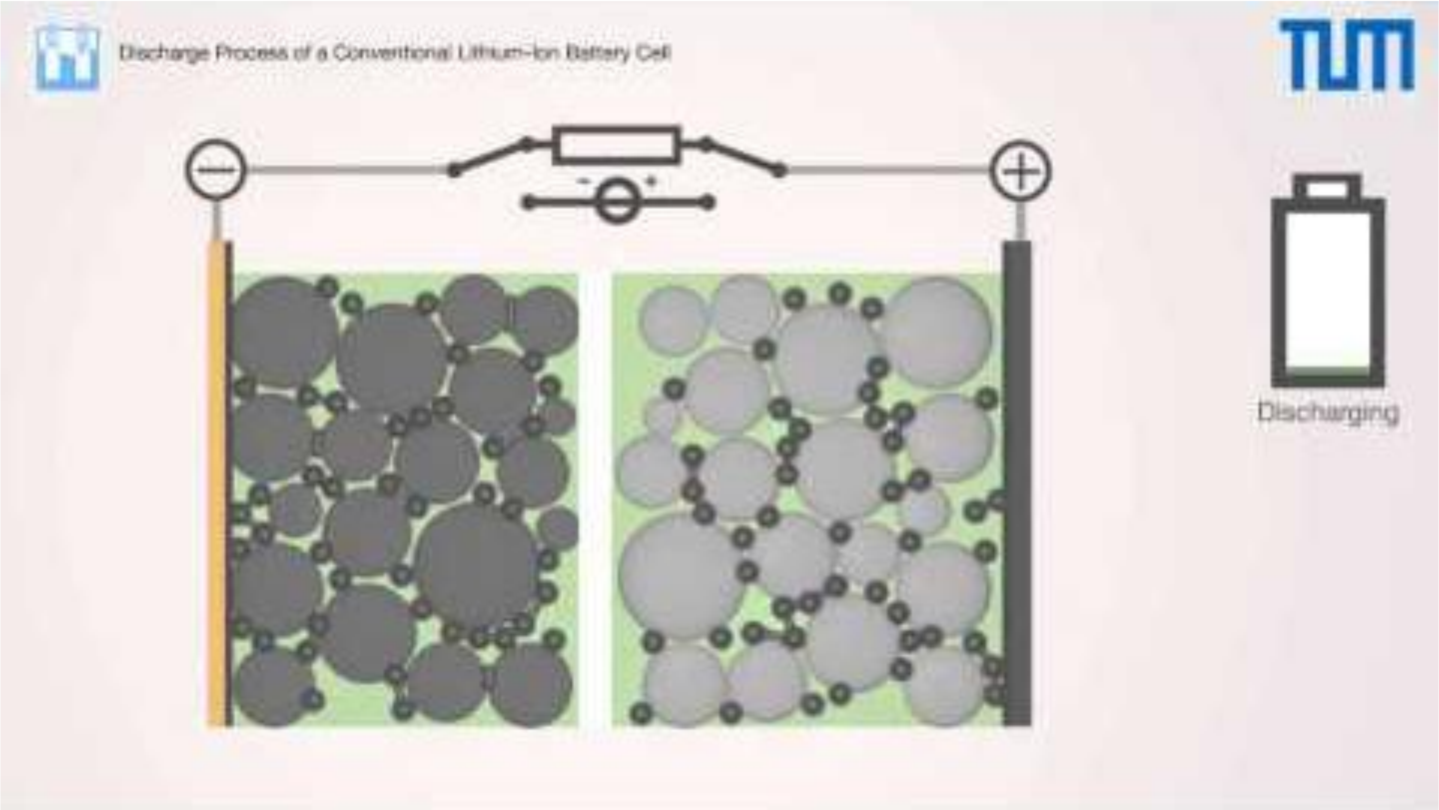
This is called an electrolyte.

$$PbO_2(s) + H_2SO_4(aq) + 2H^+(aq) + 2\,e^- \rightarrow 2\,PbSO_4(s) + 2H_2O(l)\ E^\circ_{red} = +1.69\,V$$
$$PbSO_4(s) + 2\,H^+(aq) + 2\,e^- \rightarrow Pb(s) + H_2SO_4(aq) \qquad E^\circ_{red} = -0.35\,V$$
$$PbO_2(s) + Pb(s) + 2H_2SO_4 \rightarrow 2\,PbSO_4(s) + 2\,H_2O(l) \qquad E^\circ_{cell} = +2.04\,V$$

THE UNIVERSITY OF UTAH

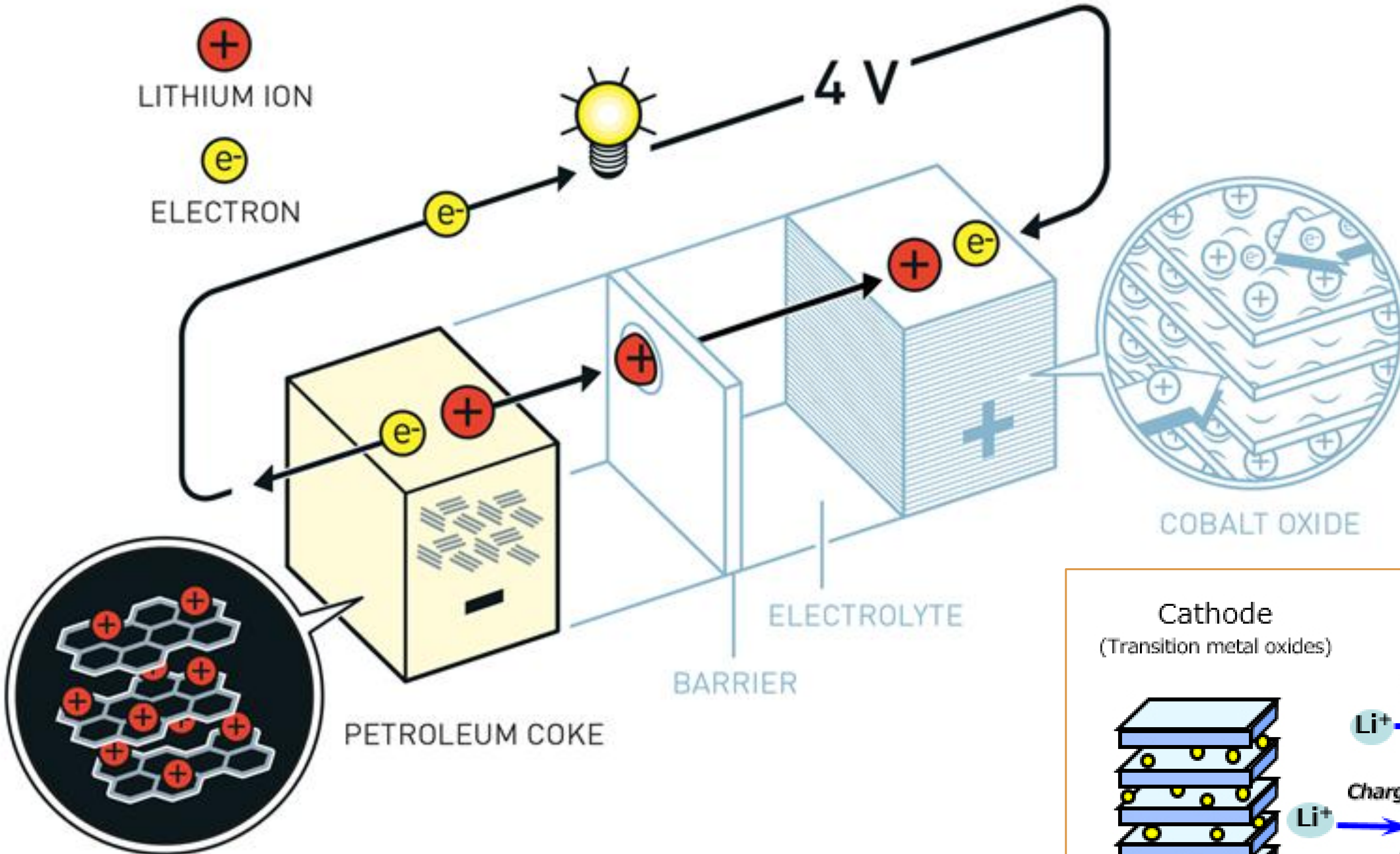
Department of Chemistry
COLLEGE OF SCIENCE | THE UNIVERSITY OF UTAH

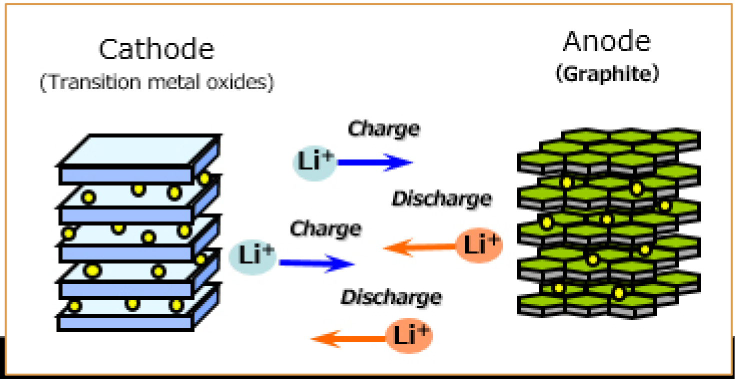
State-of-Art Battery: Li-ion



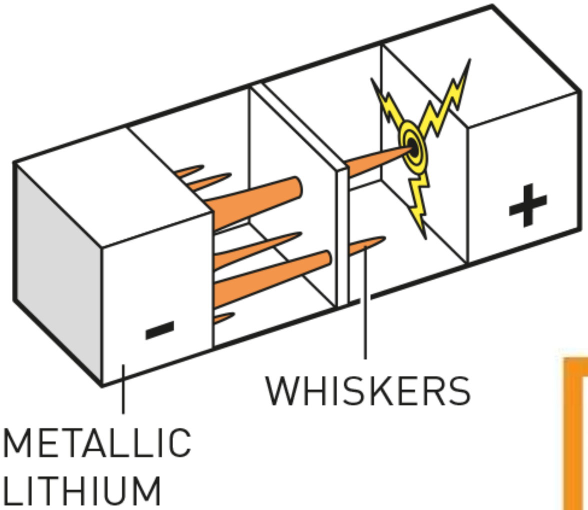
What things can be improved?

Layered Structures of Anode & Cathode

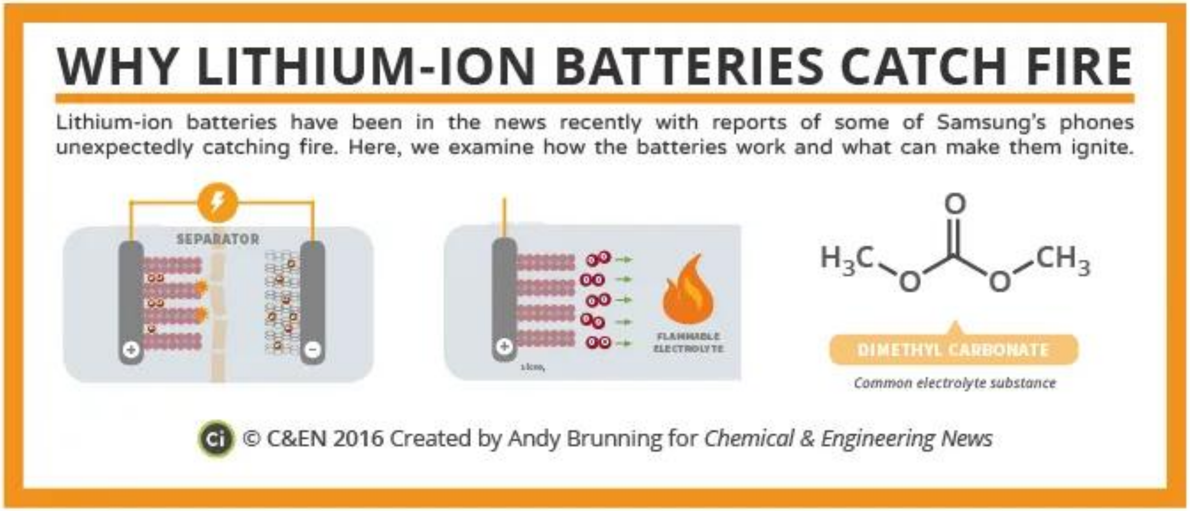




Li-ion Batteries: Flammable, Toxic



Short-circuits & gets really hot!

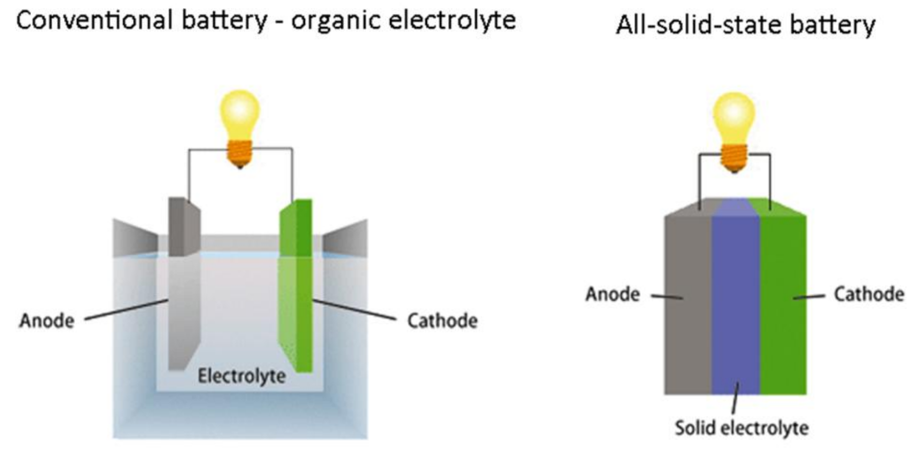


What things can be improved?

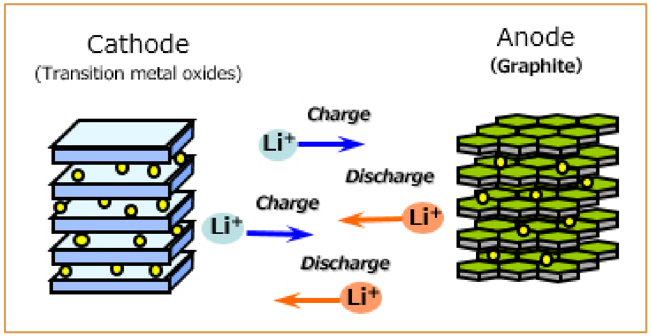
- Electrolyte
    - Aqueous solutions
    - Non-aqueous solutions
    - Solid-state electrolytes
- Binder
    - Binder-free
- Valency of the Ion
- Materials: Anode/Cathode
    - Expansion
    - SEI Layer
- Size

Research: Electrolyte

- Aqueous solutions (water: 1.23 V, non-toxic, non-flammable)
- Non-aqueous solutions (current: 4V, toxic, flammable)
- Solid-state electrolytes

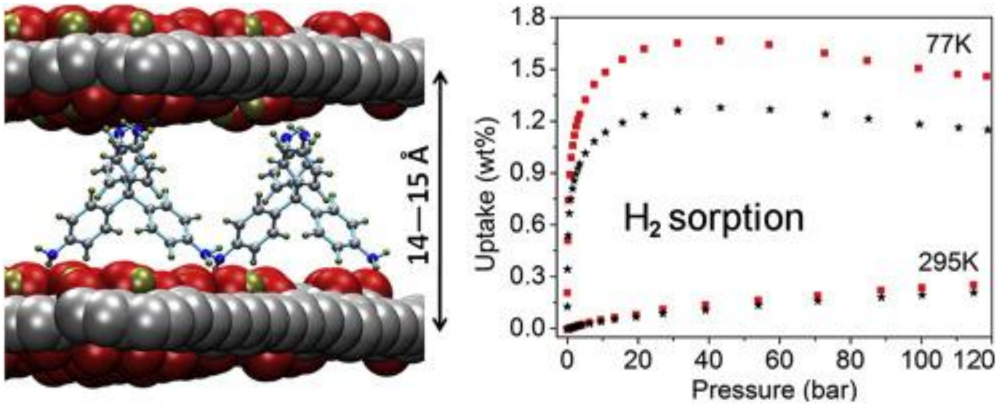


Research: Different Ions



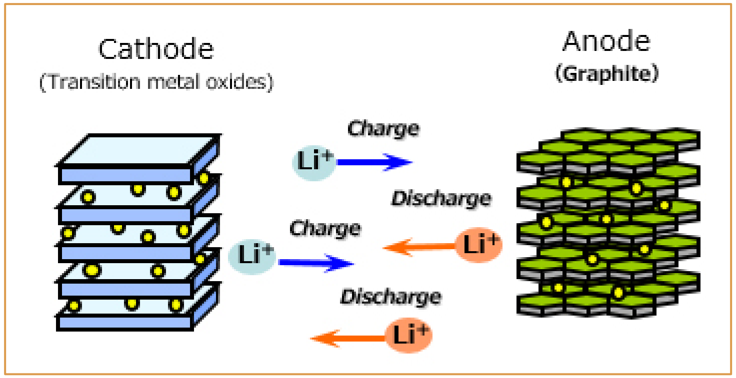
- Single-valent:
  - Li → Li^{+} + e^{-}
- Multivalent: *Higher Energy Density*
  - Mg → Mg^{2+} + $2e^{-}$ ….but larger radius!
  - Al → Al^{3+} + $3e^{-}$

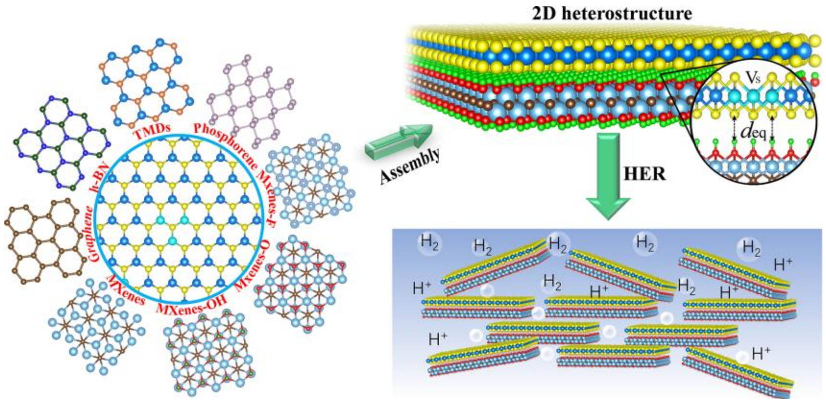
<u>Pillaring:</u>



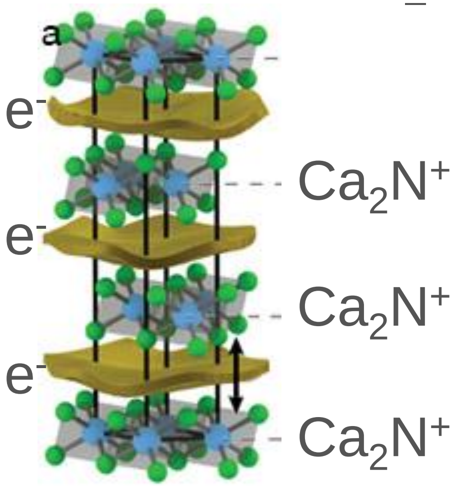
<u>Carbon</u>, vol <u>120</u>, (2017) 145-156.

Materials: Anode/Cathode



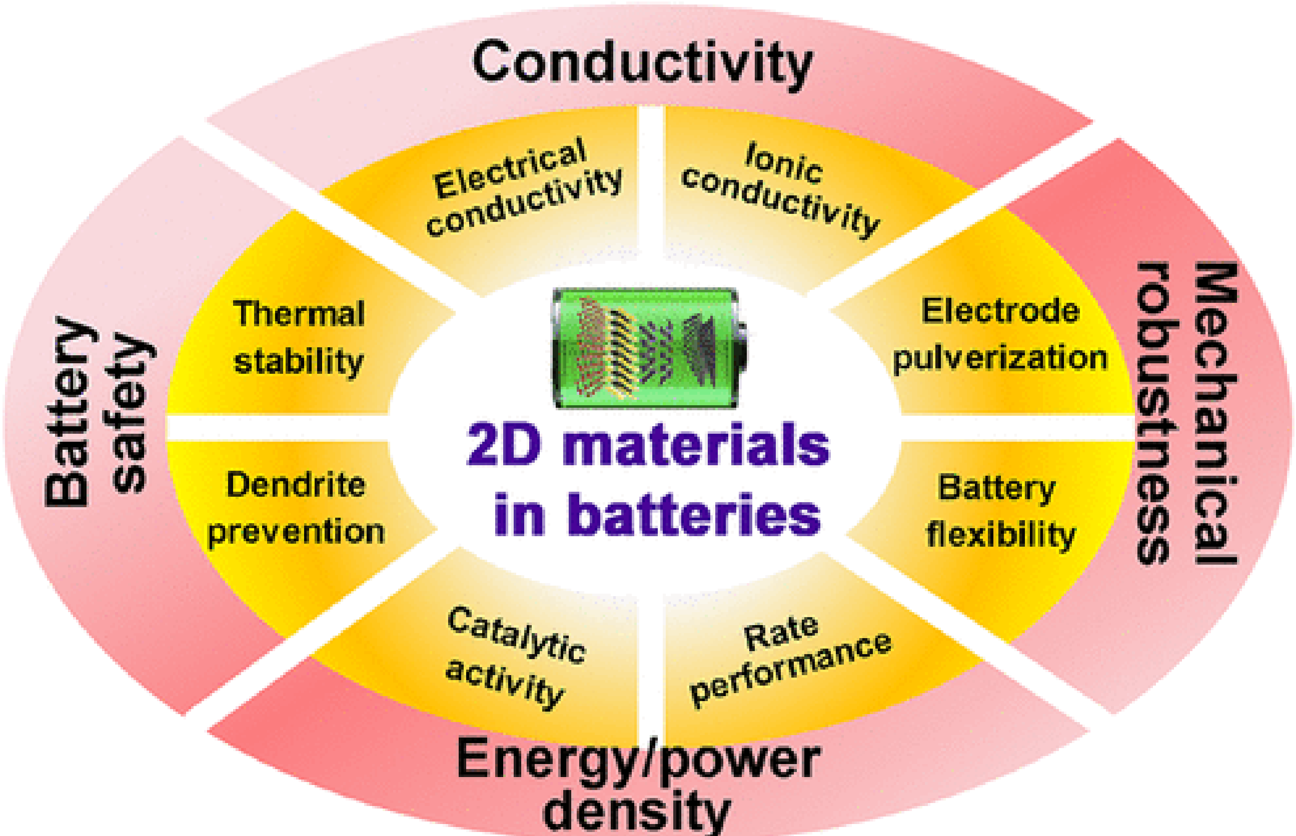


Electrides: Ca_2N



J. Am. Chem. Soc. 2016, 138, 49, 16089−16094

2D Materials to Address Li Battery Challenge



ACS Nano 2020, 14, 3, 2628−2658

References

- **C&EN's Newsletter**
  - Annual C&EN's Year in Chemistry
  - C&EN's Trailblazers (2020)
    - List of 20 entrepreneur Women
- **ACS Newsletter (Member or Archive)**
  - Annual ACS Molecule of the Year
  - Annual ACS Heroes of Chemistry
- For students: **Science Focus Newsletter**

ACS Heroes of Chemistry (2022)

"…industrial chemical scientists whose work has led to the development of successful commercialized products ingrained with chemistry for the benefit of humankind."

Congratulations to the 2022 Heroes of Chemistry!

This year's inductees into the Heroes of Chemistry scientific hall of fame include teams that developed products that have led to significant advancements in dental cements, sustainable packaging, breast cancer treatments, and formulations that protect against or treat COVID-19. Sponsored by the Committee on Corporation Associates, ACS has bestowed this honor annually since 1996.

HEROES of CHEMISTRY

The following teams will be honored at a special ceremony taking place in Washington, DC on September 29 as Heroes of Chemistry for 2022:

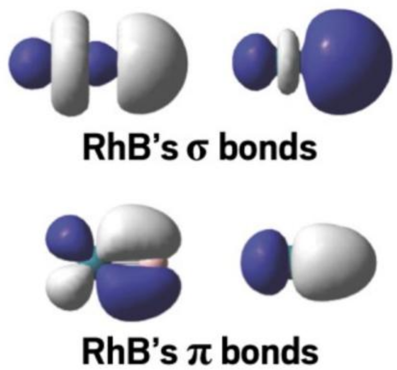
- **3M: RelyX™ Unicem and Universal Dental Cements** have simplified dental-surgery workflows and cause virtually no post operative sensitivities.
- **Dow: EliteTM and Innate™ sustainable packaging ranges.** These enhanced polyethylenes have applications ranging from flexible food packaging to heavy-duty industrial shipping sacks.
- **Eli Lilly: Verzenio® (abemaciclib)** is a selective CDK4 and CDK6 inhibitor, approved by the US Food and Drug Administration, for treating advanced and metastatic as well as high-risk early breast cancers.
- **Merck: Lagevrio (molnupiravir),** novel antiviral Covid-19 treatment FDA approved for emergency use in Dec. 2021.
- **Moderna: Spikevax™ mRNA-1273 SARS-CoV-2** vaccine first used in the U.S. in December 2020 for individuals 18 and over.
- **Pfizer: Paxlovid™** granted emergency use by the FDA in Dec. 2021 for the treatment of mild to moderate COVID-19.

Nominations for the 2023 awards will open in November. Visit the Heroes of Chemistry website for more information about the 2022 honorees, eligibility and nomination details, and profiles of past recipients. Please send any questions to chemhero@acs.org. Congratulations to the 2022 winners for their hard work and dedication!

ACS Molecule of the year

2020

BORON MAKES QUADRUPLE BOND



Credit: *J. Phys. Chem. Lett.*

These molecular orbitals (purple and silver) show the two σ bonds and two π bonds that make up the quadruple bond in rhodium boride (aquamarine = Rh; pink = B).

For more than a decade, chemists have thought that rhodium boride contains a triple bond. Using vibrational spectroscopy and theoretical calculations, researchers at Brown University discovered that the bond is likely a **quadruple bond** instead (*J. Phys. Chem. Lett.* 2020, DOI: **10.1021/acs.jpclett.9b03484**).

2021

MOLECULE GOES TO INFINITY AND BEYOND

Infinitene

Researchers at Nagoya University fused 12 benzene rings to make **a molecule that loops like an infinity symbol** (ChemRxiv 2021, DOI: **10.33774/chemrxiv-2021-pcwcc**). In X-ray crystal structures, only 3.192 Å separated the upper and lower benzene rings where the molecule, called infinitene, crosses over itself. Through computational studies, the chemists confirmed that infinitene's π electrons are delocalized within individual benzene rings, not across the entire molecule. The study, which appeared as a preprint, has not yet been peer-reviewed.