

technocamps



UNDEB EWROPEAIDD
EUROPEAN UNION



Llywodraeth Cymru
Welsh Government

Cronfa Gymdeithasol Ewrop
European Social Fund



Prifysgol
Abertawe
Swansea
University



CARDIFF
UNIVERSITY
PRIFYSGOL
CAERDYDD



PRIFYSGOL
BANGOR
UNIVERSITY



Cardiff
Metropolitan
University

Prifysgol
Metropolitan
Caerdydd

it.wales



PRIFYSGOL
ABERYSTWYTH
UNIVERSITY

PRIFYSGOL
Glyndŵr
Wrecsam

PRIFYSGOL
Wrexham
glyndŵr
UNIVERSITY

University of
South Wales
Prifysgol
De Cymru

Modelling Molecules



Activity: What Is Modelling?

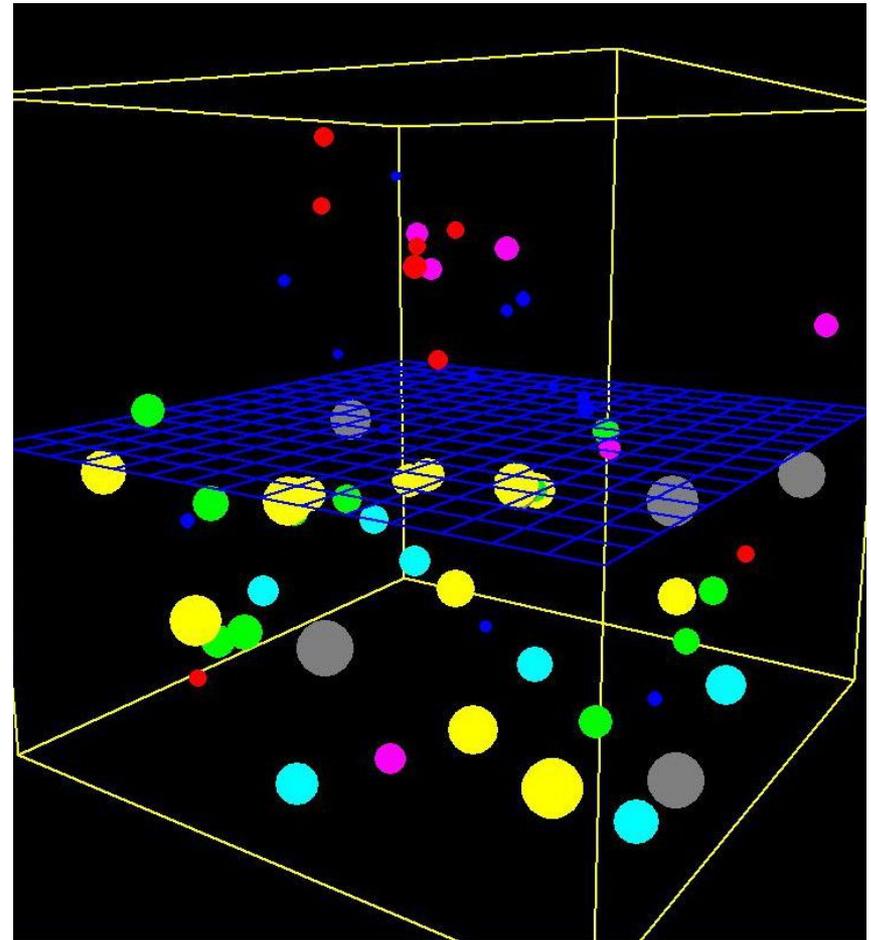
Write in your workbooks what you think Modelling is in the context of computer science.



Modelling

Modelling is the process of building a simpler version of real-world things in order to understand them better.

Today we will be looking particularly at modelling how atoms move and behave in different states of matter.



What Is an Atom?

An Atom is the building block of nature. Just like houses are (usually) built with bricks, and old ships were made with planks of wood.

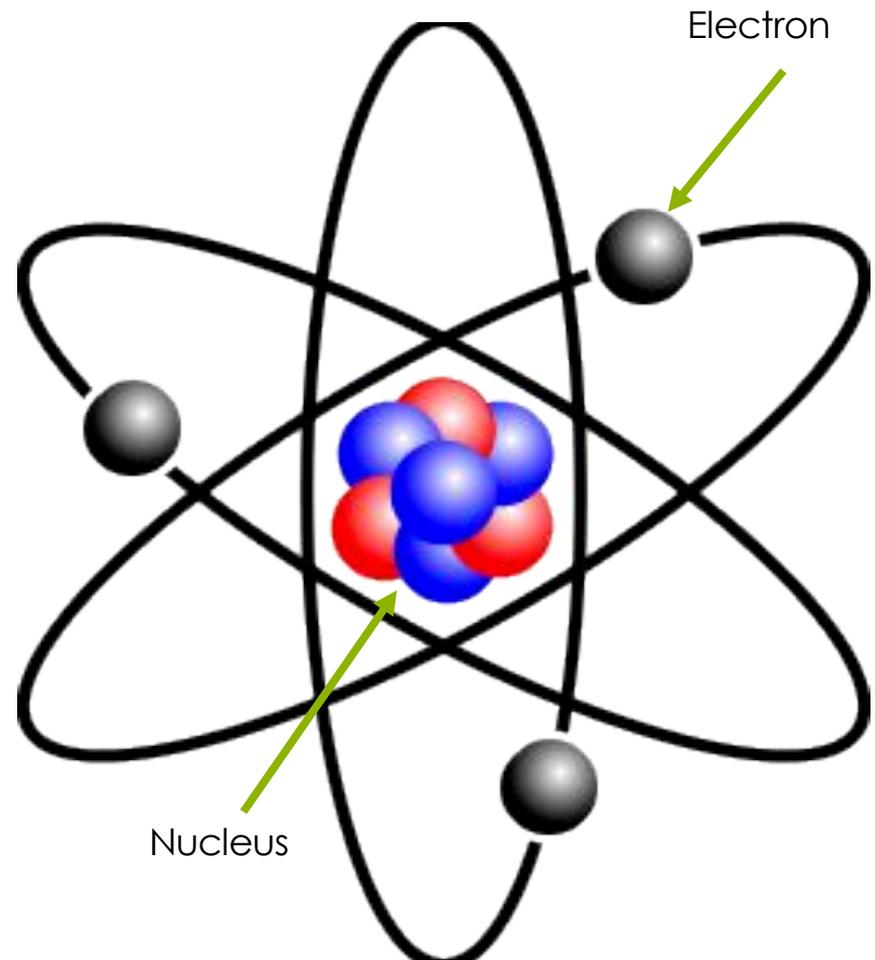
Atoms are the tiny pieces that make up every material, every liquid, almost everything in the entire universe.



What Does an Atom Look Like?

An atom can be thought of as two main parts, the nucleus in the centre, and the electron shells around it.

However, this image is not to scale and doesn't give a good idea of the size of an atom.

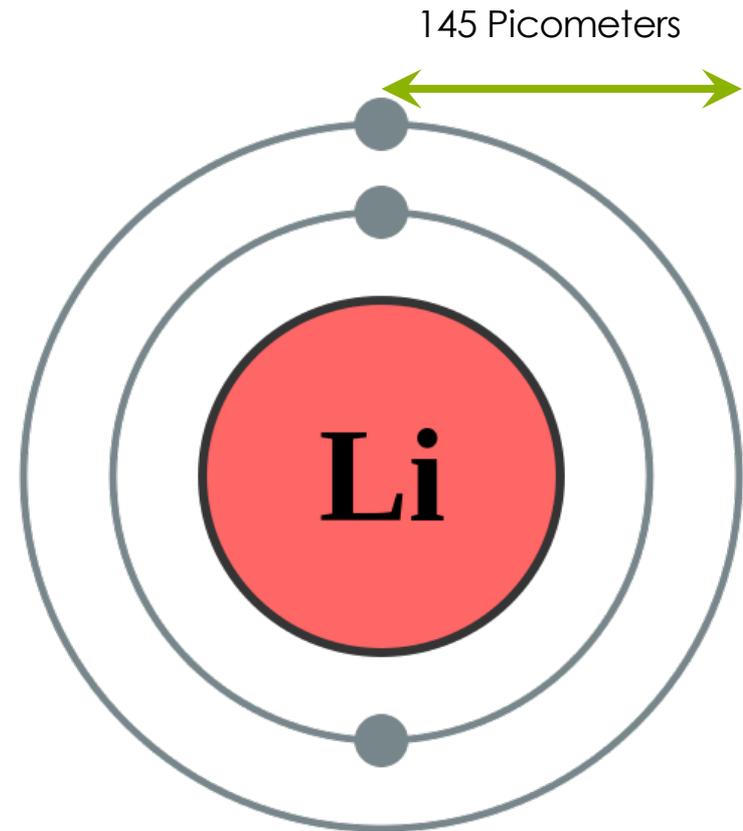


How Big Is an Atom?

A Hydrogen atom has a radius of around **25 picometers**. This is incredibly small!

In a metre there are 1,000,000,000,000 picometres.

A picometre is much smaller than our eyes can see, so we can never see atoms (unless using a very powerful and clever microscope.)

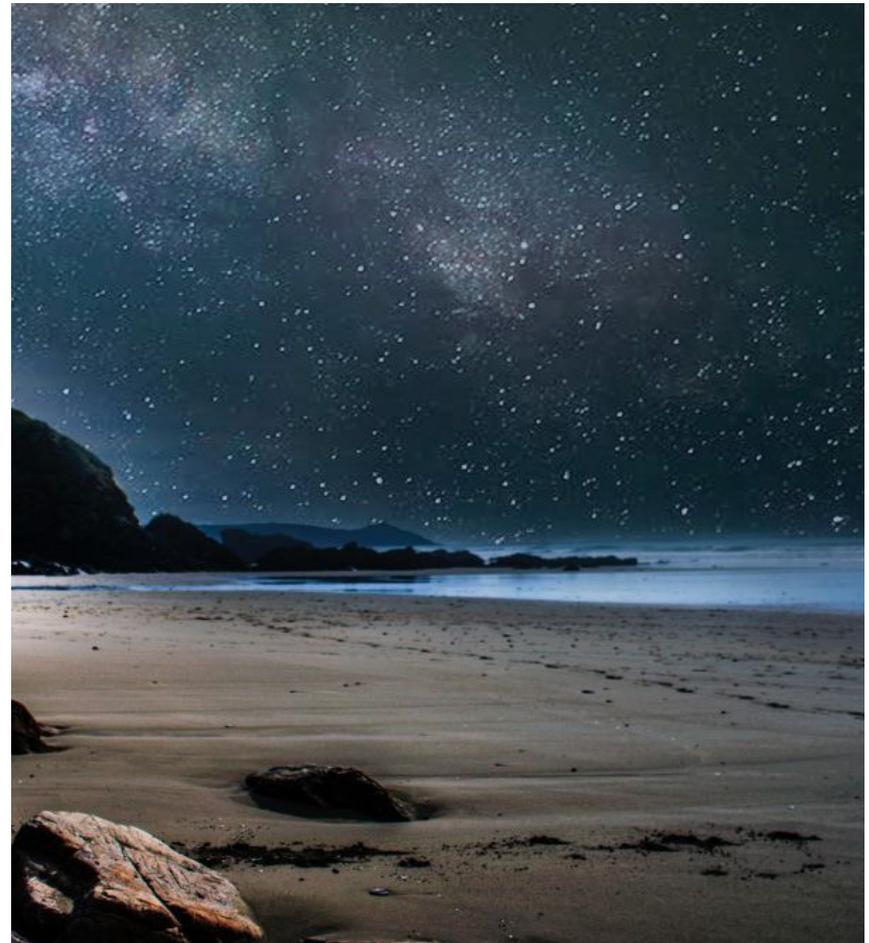


A lithium atom is slightly bigger as it has two electron shells.

A Better Idea of The Size of Atoms

A **single grain of sand** contains around 50 quintillion atoms. i.e. **50,000,000,000,000,000,000 atoms.**

There are between 5-10 times more stars in the universe than grains of sand on the Earth, but there are more atoms in a single grain of sand than stars in the entire universe.



States of Matter

Now that we know that everything is made up of atoms, we can explain different states of matter by looking at how these atoms behave.

The 3 (main) States of Matter are:

States of Matter

Now that we know that everything is made up of atoms, we can explain different states of matter by looking at how these atoms behave.

The 3 (main) States of Matter are:

Solid

Liquid

Gas

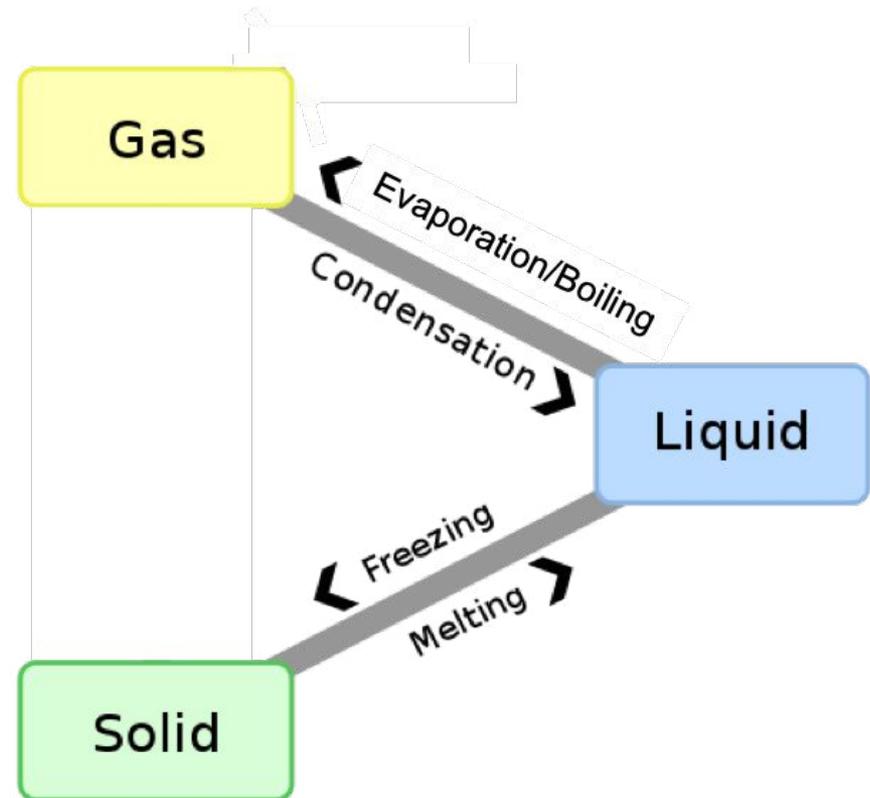


Phase Transitions

Elements can be found in the 3 states of matter depending on the temperature (or pressure).

Each element has its own melting and boiling point.

Compounds such as water will have different melting and boiling points to the elements Oxygen and Hydrogen.



Boiling and Melting Points

What is the Melting/Freezing point of water?

What is the Boiling point of water?

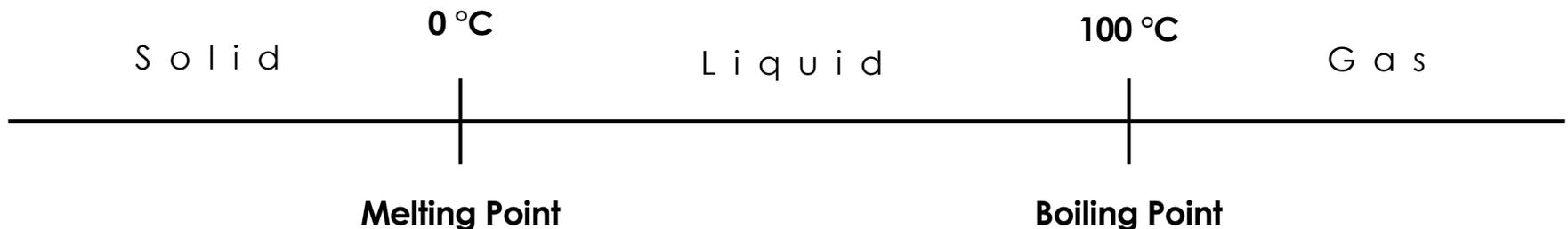
Boiling and Melting Points

What is the Melting/Freezing point of water?

0 °C

What is the Boiling point of water?

100 °C



Activity: Boiling and Melting Points

In your workbooks, draw and complete the following diagram for **water**:



In which state is **water** at the following temperatures:

1. 70 °C
2. 121 °C
3. -20 °C

Activity: Boiling and Melting Points

In your workbooks, draw and complete the following diagram for **mercury**:



In which state is **mercury** at the following temperatures:

1. 70 °C
2. 121 °C
3. -20 °C

Activity: Boiling and Melting Points

In your workbooks, draw and complete the following diagram for **oxygen**:



In which state is **oxygen** at the following temperatures:

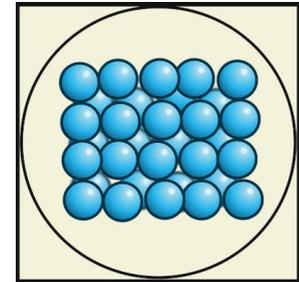
1. $-10\text{ }^{\circ}\text{C}$
2. $-200\text{ }^{\circ}\text{C}$
3. $-250\text{ }^{\circ}\text{C}$

How Do Atoms Move?

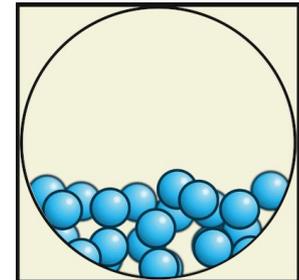
Atoms are always moving, but depending on certain variables such as temperature, they can move in different ways.

In each of the 3 states of matter, atoms will behave differently.

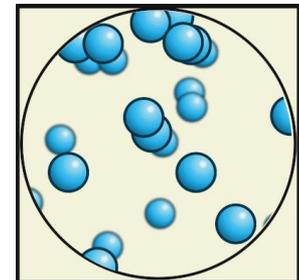
Solid



Liquid



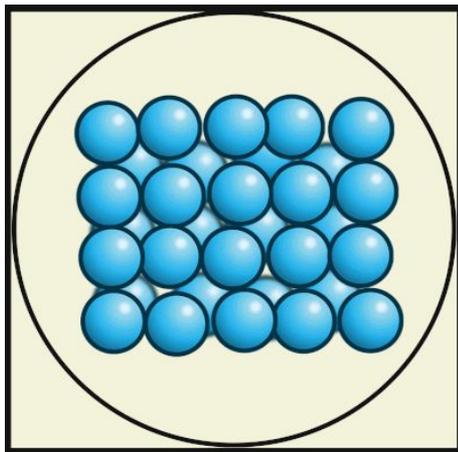
Gas



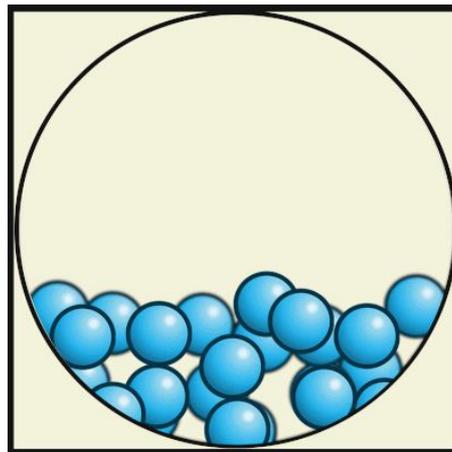
Activity: How Do Atoms Move?

In your workbooks, write a short description of how atoms move in each state of matter. Think about their speeds, how much they move, and how much space is between the atoms.

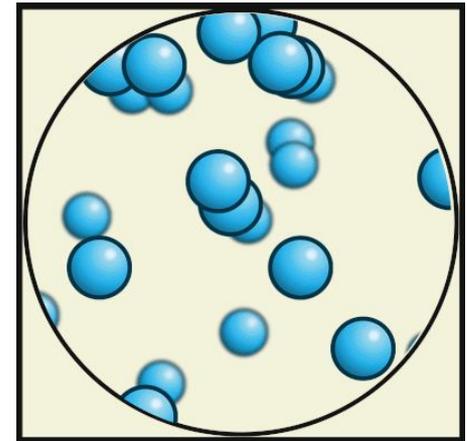
Solid



Liquid



Gas



Atom Behaviour Comparison

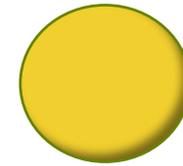
Solid	Liquid	Gas
<p>Vibrate back and forth, but remain in the same position.</p>	<p>Move around slower than a gas.</p>	<p>Move around much faster than liquid atoms.</p>
<p>Does not flow easily. Particles cannot move/slide past one another.</p>	<p>Flows easily. Particles can move/slide past one another.</p>	<p>Flows easily. Particles can move past one another.</p>
<p>Little free space between particles. Not easily compressible.</p>	<p>Little free space between particles. Not easily compressible.</p>	<p>Lots of free space between particles. Compressible.</p>

What Is a Molecule?

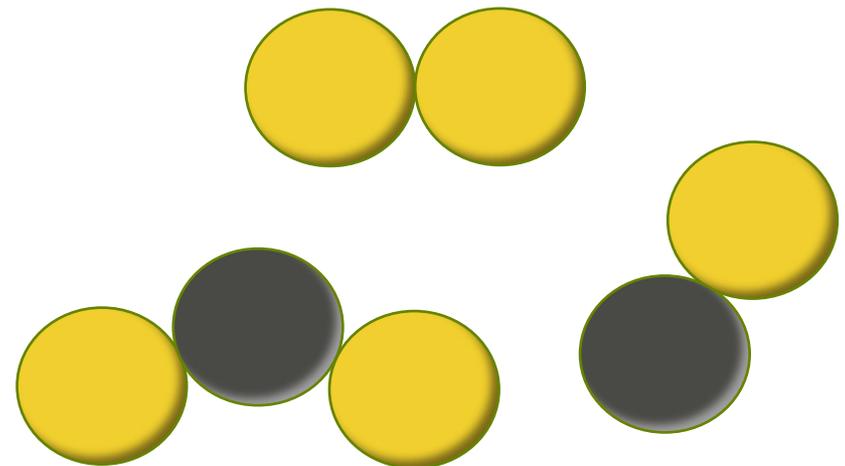
A molecule is **2 or more atoms bonded together**. They could be the same or different elements.

It's important that we understand the difference in general, however **when we're only concerned with the movement** of these we can **simplify** our model to just **be plain, coloured circles**.

Atom:

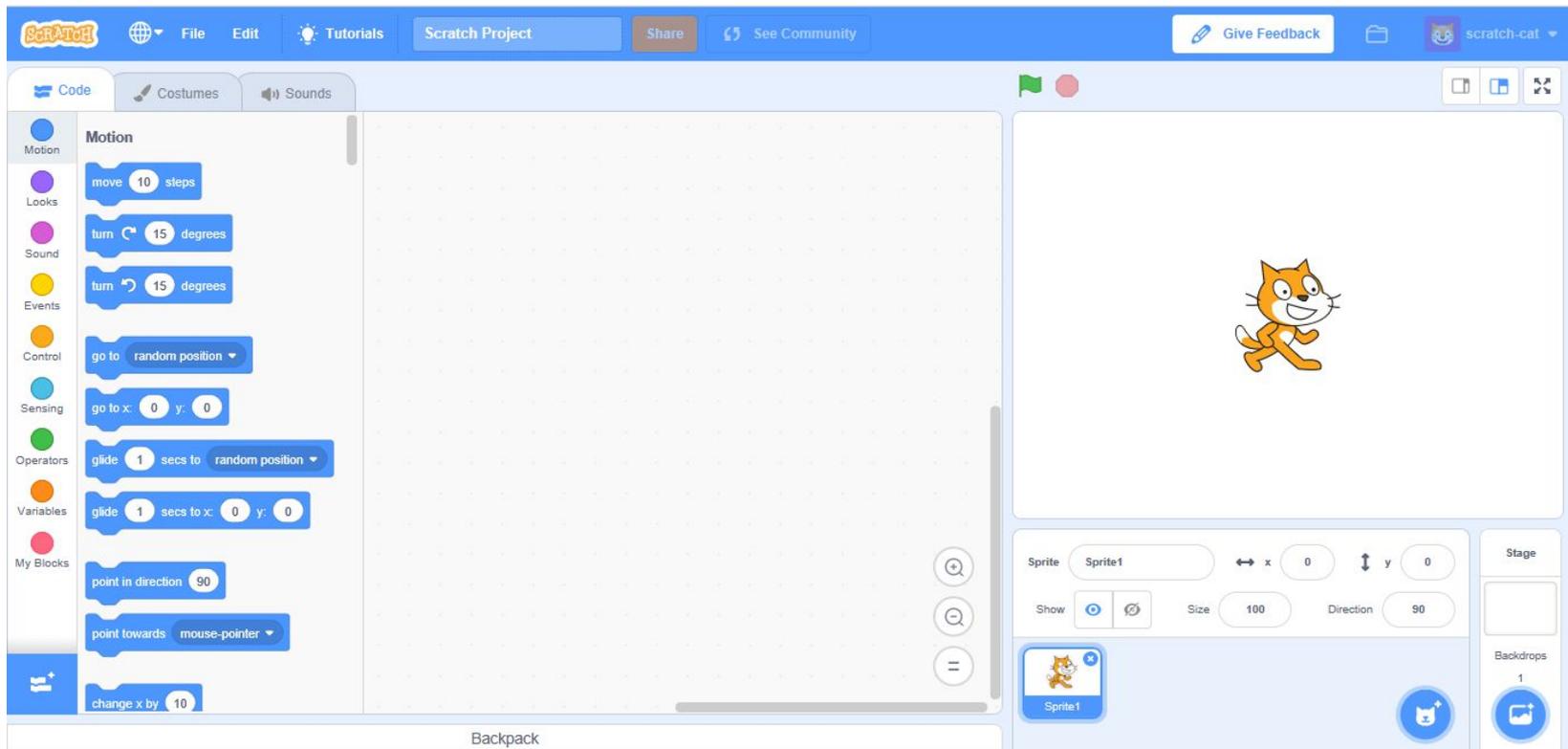


Molecules:



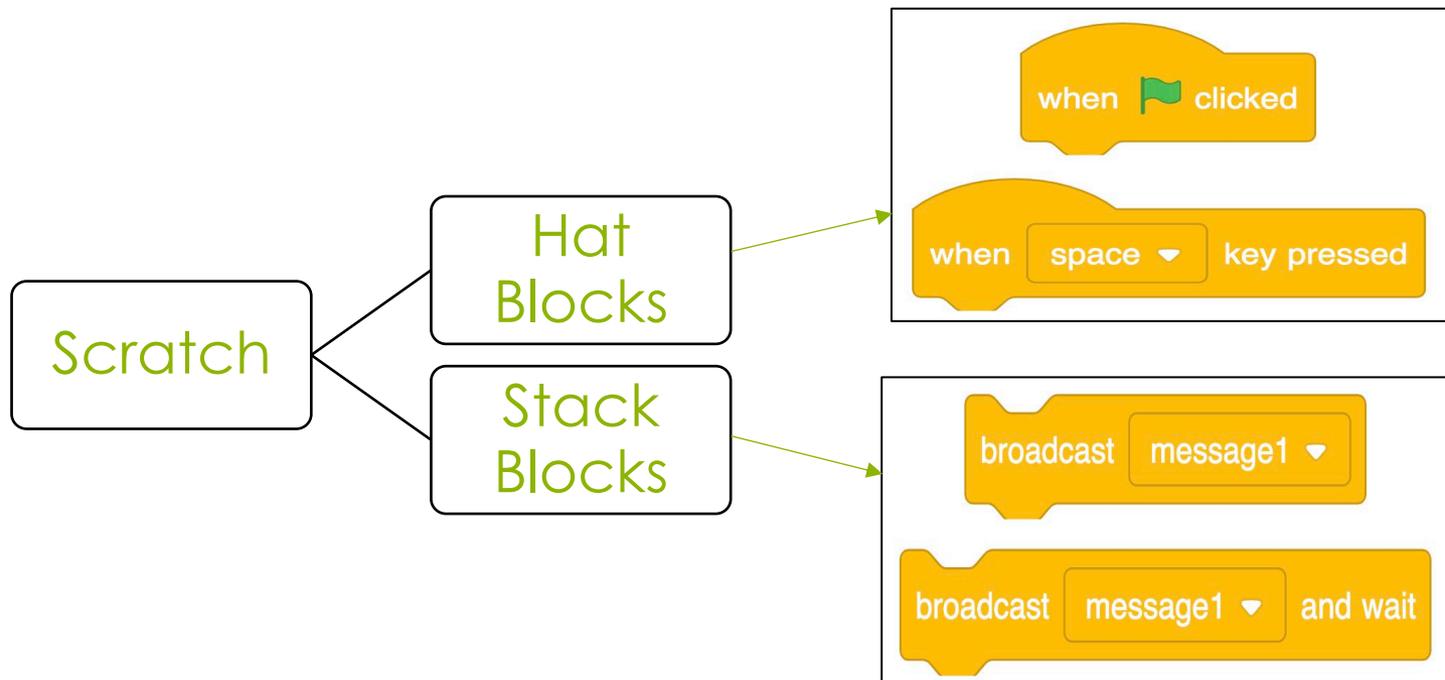
Scratch - States of Matter

We will now create a Scratch program to simulate water at different temperatures.



Scratch

- Drag and drop blocks to give instructions
- Easy to create games and other useful programs
- User friendly



Scratch Basics

The image shows the Scratch web interface with several key components highlighted by green callout boxes:

- Blocks Palette:** Located on the left side, it contains various colored blocks categorized by function: Motion (blue), Looks (purple), Sound (pink), Events (yellow), Control (orange), Sensing (light blue), Operators (green), Variables (red), and My Blocks (pink).
- Sprite Costume Area:** Located at the top left of the workspace, it allows users to select and manage different costumes for their sprite.
- Scripting Area:** The central workspace where users can drag and drop blocks to create scripts for their sprites.
- Background List:** Located at the bottom right, it provides a selection of different background images for the stage.
- Stage:** The main area where the sprite's actions are performed and the background is displayed.
- Sprites List:** Located at the bottom left, it shows a list of all sprites currently on the stage, including their names and positions.

A central green callout box labeled "Blocks" points to the Control category in the Blocks Palette.

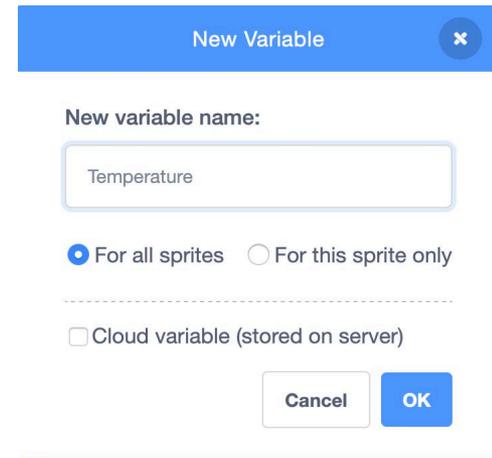
Activity: Taking a User Input

First, we need our program to ask the user for a temperature.

We then want to store their answer as a variable named something like “temperature”

To create a variable:

1. Click the orange variables category.
2. Click Make a new variable.
3. Name your variable and click Ok.



The image shows a 'New Variable' dialog box with a blue header bar containing the title 'New Variable' and a close button (an 'x' in a circle). Below the header, the text 'New variable name:' is followed by a text input field containing the word 'Temperature'. Underneath the input field, there are two radio button options: 'For all sprites' (which is selected) and 'For this sprite only'. A dashed horizontal line separates these options from a checkbox labeled 'Cloud variable (stored on server)'. At the bottom right of the dialog, there are two buttons: 'Cancel' and 'OK'.

If Statements

An if statement is a way of making a selection in programs.

By checking if something is true or not, we can make the program do different things depending on the outcome.

For example:

If you have blue eyes, **then** raise your hand.

If it is raining, **then** wear a coat.

If the temperature is less than 5°C, **then** turn on the heating.

Activity: True or False

Write whether the following statements would be true or false (remember that “>” means “is more than” and “<” means “is less than”):

Question	Statement	True or False
1.	$5 = 5$	_____
2.	$7 \times 3 = 24$	_____
3.	$5 > 3$	_____
4.	$5 < 3$	_____
5.	$0 < 0$	_____

Activity: True or False

Write whether the following statements would be true or false (remember that “>” means “is more than” and “<” means “is less than”):

Question	Statement	True or False
1.	$5 = 5$	True
2.	$7 \times 3 = 24$	False
3.	$5 > 3$	True
4.	$5 < 3$	False
5.	$0 < 0$	False

Activity: Checking the State of the Water

We want our program to work out if water is Solid, Liquid or Gas at the temperature entered.

We can do this by using 3 **if-then** blocks, each one checking if the water is in each state of matter. We can then broadcast a message for each state to tell our particles how to behave.

When is water solid?

When is it liquid?

And a gas?

Activity: Checking the State of the Water

We want our program to work out if water is Solid, Liquid or Gas at the temperature entered.

We can do this by using 3 **if-then** blocks, each one checking if the water is in each state of matter. We can then broadcast a message for each state to tell our particles how to behave.

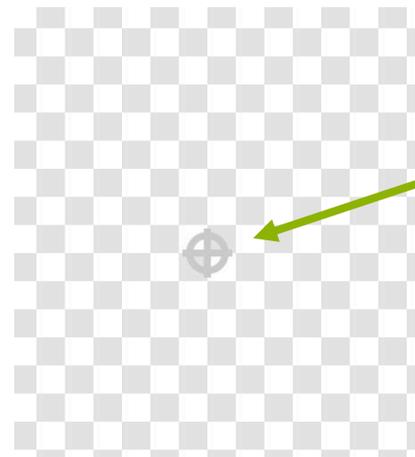
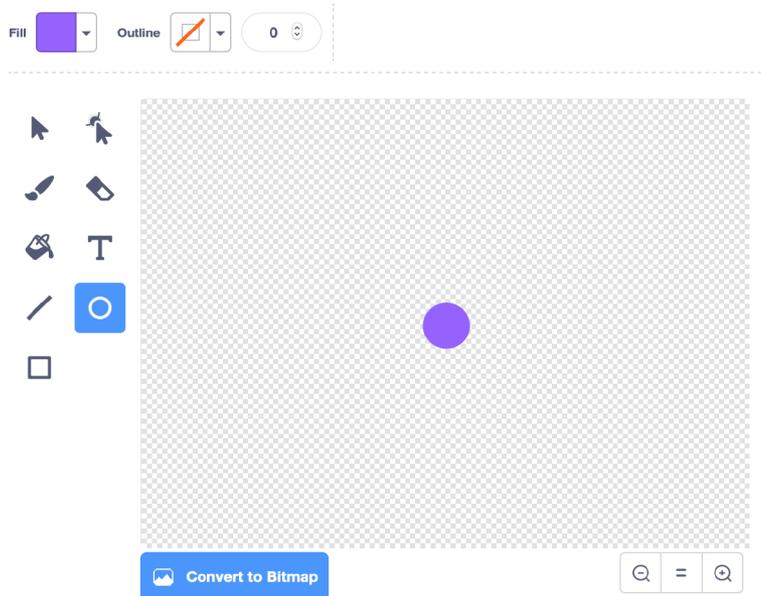
When is water solid? **When temperature < 1**

When is it liquid? **When temperature > 0 AND temperature < 100**

And a gas? **When temperature > 99**

Activity: Adding a Molecule

Create a new sprite for a particle. We can simplify it to just being a simple circle with a certain colour. (Holding the shift key when making the circle will make a perfect circle.)



Make sure you place the circle in the centre of the window on the crosshair

Activity: Movement of Molecules in a Solid

Atoms and Molecules in a solid tend to vibrate back and forth in random directions, but always remaining in the roughly the same position.

When making the molecules move you should not use glide!



Activity: Movement of Molecules in a Liquid

Atoms and Molecules in a liquid tend to move around relatively slowly (compared to in a gas) in straight lines colliding with each other.

Activity: Movement of Molecules in a Gas

Atoms and Molecules in a gas tend to move around relatively quickly (compared to in a liquid) in straight lines colliding with each other.

Activity: Duplicating Molecules

Duplicate your molecule by right clicking on the image of the sprite and selecting duplicate.

Do this as many times as you would like in order to add more molecules to the program.

Be careful: If you've duplicated sprites and then want to change the code, you will need to delete the copies and then duplicate the sprite again once you've changed the code.

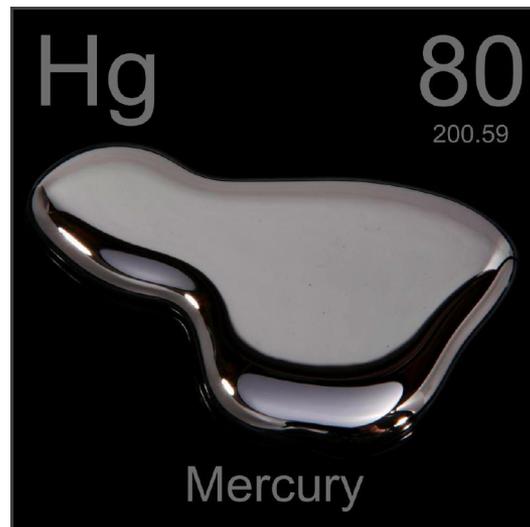
Activity: Adding a Label for the State

Add another sprite which will display which state the water is currently in. i.e. if the molecules are displaying the movement of a solid, liquid or gas.

Activity: Adjusting the Program for Mercury

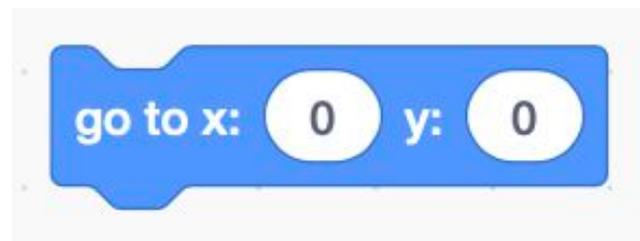
Once you have finished your program, adjust it for the element mercury. **Remember, mercury has different melting and boiling points to water.**

If you'd like to change the colour of the particles, mercury has a silver colour to it.



Activity: Improving Our Model

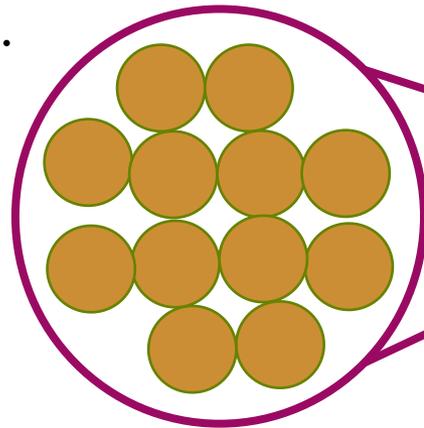
One way to improve our model would be to make the atoms/molecules clump together when they are solid. Can you think of a way to do this using the following block?



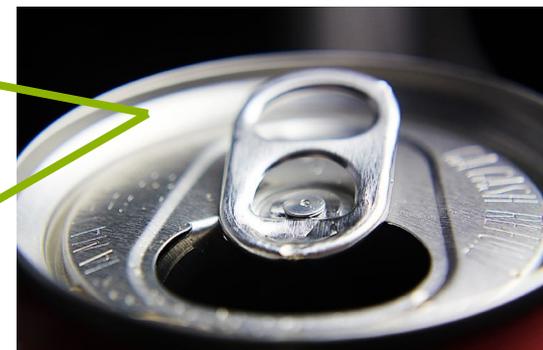
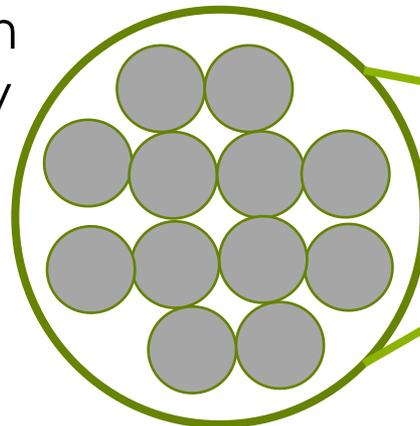
Remember, we **don't** want them to spread across the screen **randomly**.

Elements

Gold is an element made only of atoms of Gold.



Aluminium is also an element made only from atoms of aluminium.

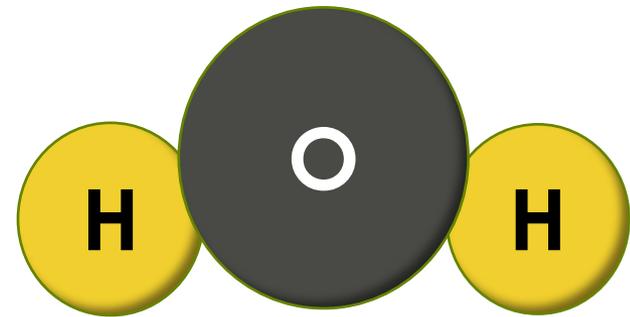


Compounds

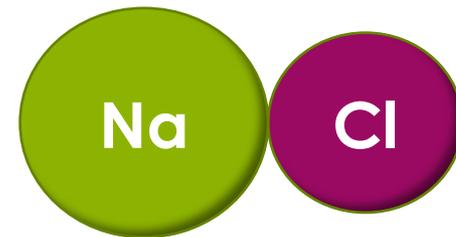
Compounds are made from two or more **different** elements, which react and bond together to form new substances.

For example, an atom of the element Oxygen and two atoms of Hydrogen bond together to form Water.

Table Salt is made of an atom of Sodium and an atom of Chlorine.



Water



Sodium Chloride

Mixtures

A chemical mixture contains elements and/or compounds that are not chemically bonded together.

Coca Cola is a mixture of different compounds and molecules.

It contains many different compounds and elements which are not bonded together (mostly sugar!)



Element, Compound, or Mixture?

Iron

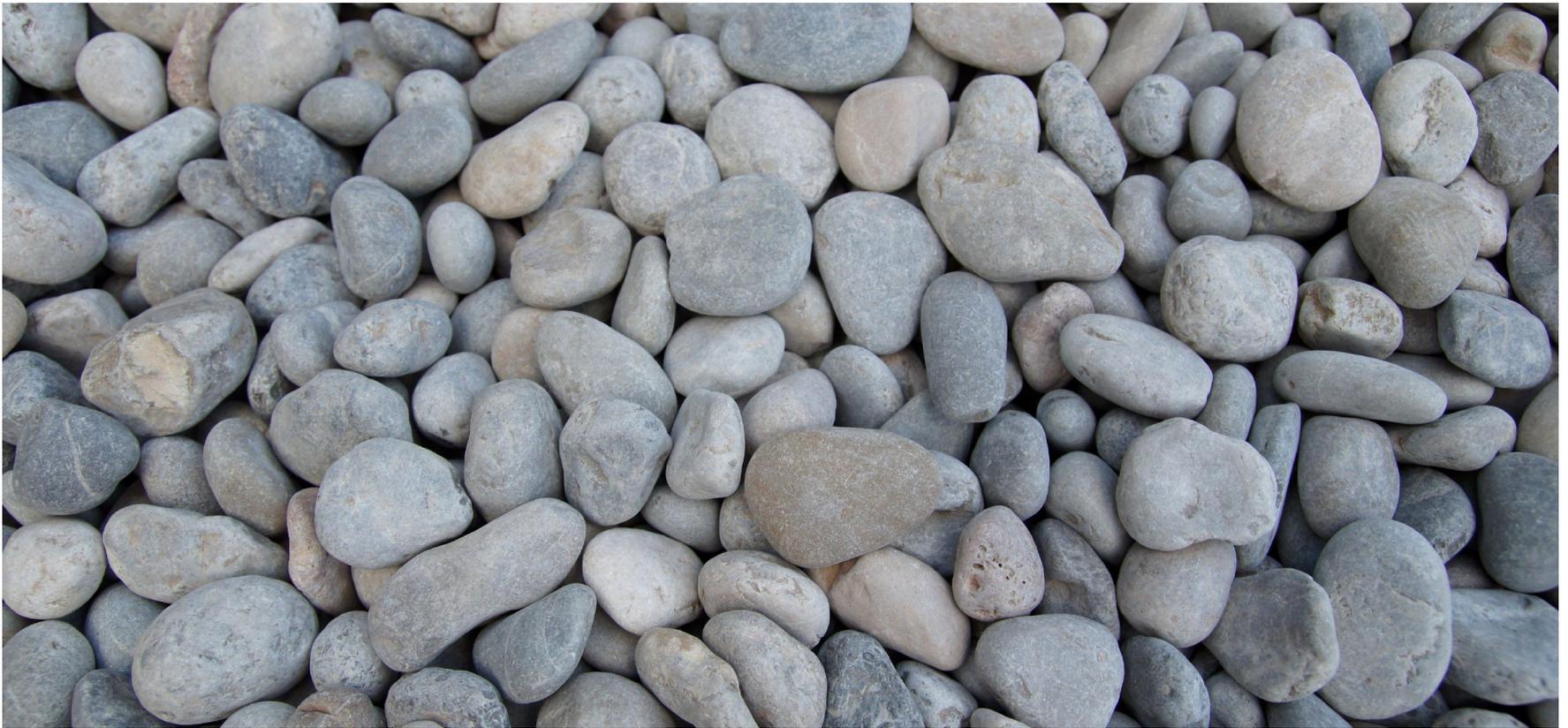


Element, Compound, or Mixture? Smoothie



Element, Compound, or Mixture?

Rocks



Element, Compound, or Mixture?

Table Sugar (Only Glucose)



Glucose is made up of Carbon, Hydrogen and Oxygen.

Element, Compound, or Mixture? Diamond



Element, Compound, or Mixture?

Neon



Element, Compound, or Mixture? Salad



Element, Compound, or Mixture?

Sand

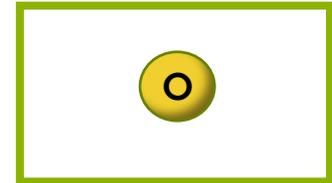


Activity: Atoms, Molecules and Compounds

Match the following terms with their definitions and examples:

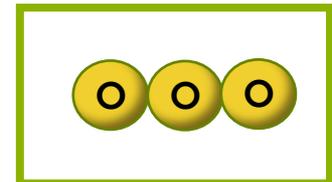
Compound

Consists of two or more different elements **and/or** compounds.



Mixture

A group of atoms bonded to each other. They can be the **same or different** types of atoms.



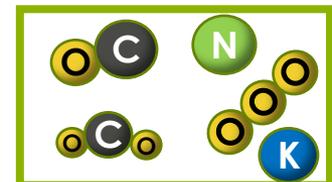
Atom

A molecule of atoms of two or more **different** elements bonded together.



Molecule

The smallest particle of a chemical element that can exist.



Solution:

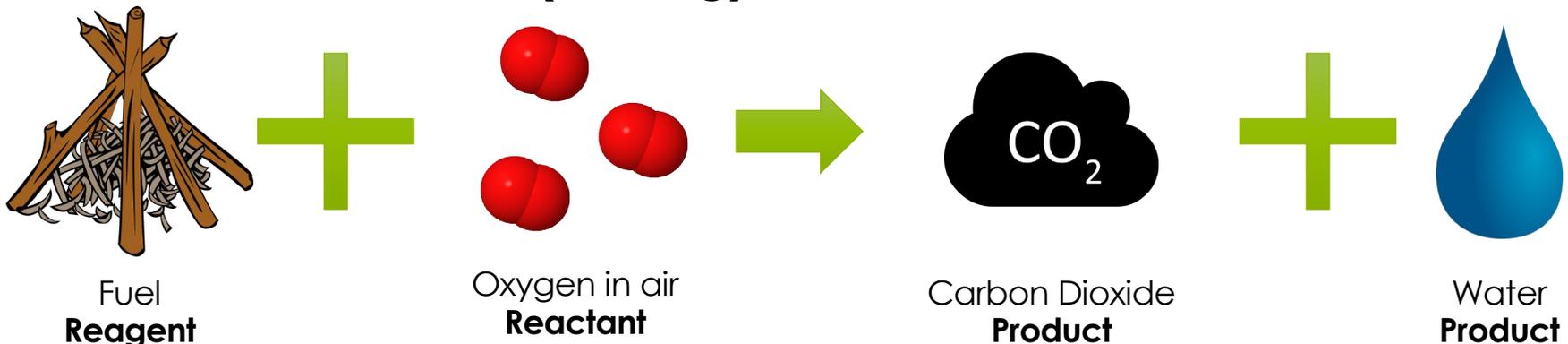
Compound	A molecule of atoms of two or more different elements bonded together.	
Mixture	Consists of two or more different elements and/or compounds.	
Atom	The smallest particle of a chemical element that can exist.	
Molecule	A group of atoms bonded to each other. They can be the same or different types of atoms.	

Chemical Reactions

A chemical reaction is a process where two different substances or elements are mixed together.

Chemical reactions occur when two or more substances are mixed together to form a new material. This change happens because **reagents** and **reactants** are mixed together.

Combustion Reaction (Burning):

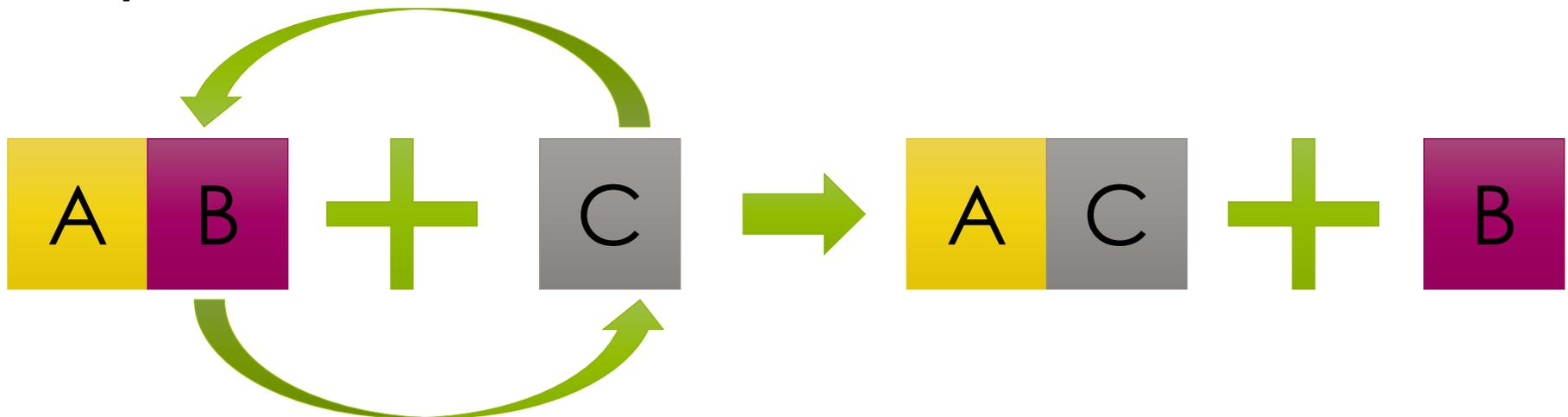


Displacement Reactions

Displacement reactions occur when one or more compounds take away a substance from another compound.

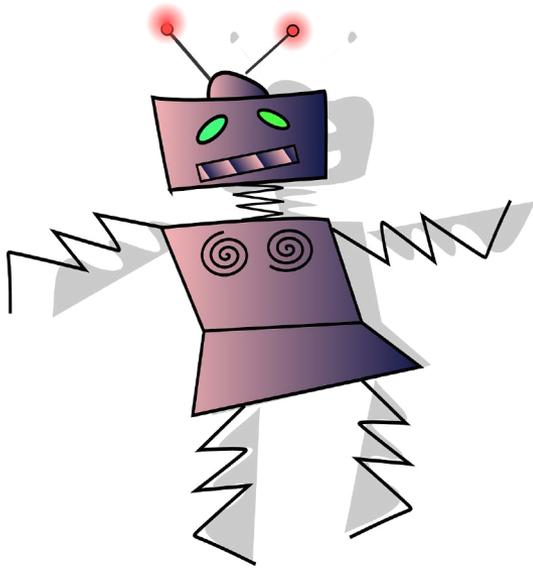
This can occur as a single displacement, where only one substance is taken away, or as a double displacement, where two substances are swapped.

Displacement Reaction:



Displacement Disco

AI the dancing robot goes to a disco looking to improve his dancing:



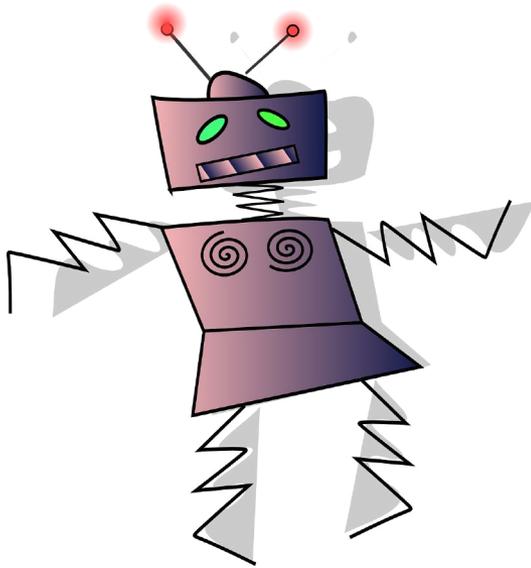
AI



Bob

Displacement Disco

AI is very impressed by Bob's dance and stands next to him trying to copy it:



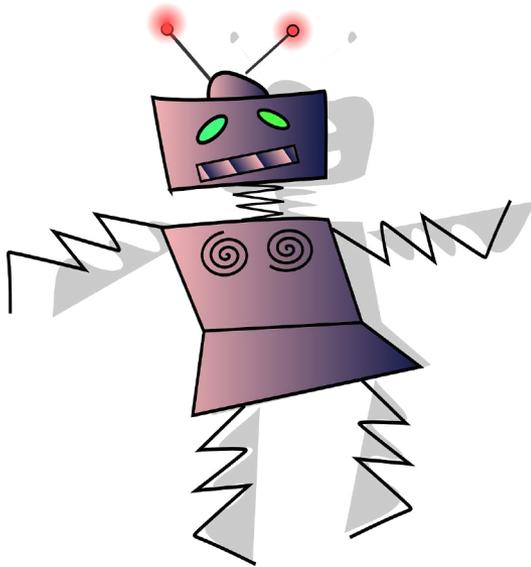
AI



Bob

Displacement Disco

Whilst AI is happily learning his new dance, he notices CJ who is doing a very unusual new dance:



AI



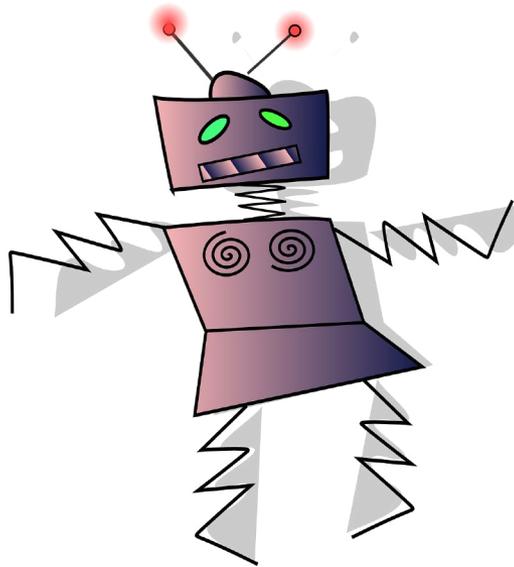
Bob



CJ

Displacement Disco

AI prefers CJ's new dance and so CJ takes Bob's place and Bob is left dancing alone i.e. Bob was displaced by CJ:



AI



CJ



Bob

Gareth Bale

Gareth Bale was happily playing his football at Spurs:



Bale



Tottenham
Hotspur

Gareth Bale

However Real Madrid wanted to sign him. Real Madrid had a lot more money and were more successful:



Bale



Tottenham
Hotspur



Real
Madrid

Gareth Bale

Because Real Madrid was a more attractive club to Bale, he signed with them and Tottenham were left alone i.e Tottenham were displaced by Real Madrid:



Bale



Real
Madrid



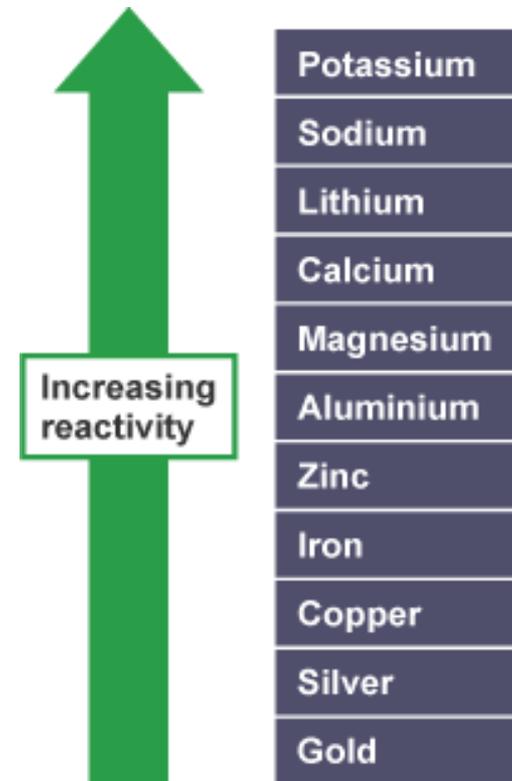
Tottenham
Hotspur

Reactivity Series

The Reactivity Series lists metals in terms of how much they react with other substances.

Metals reacting with water:

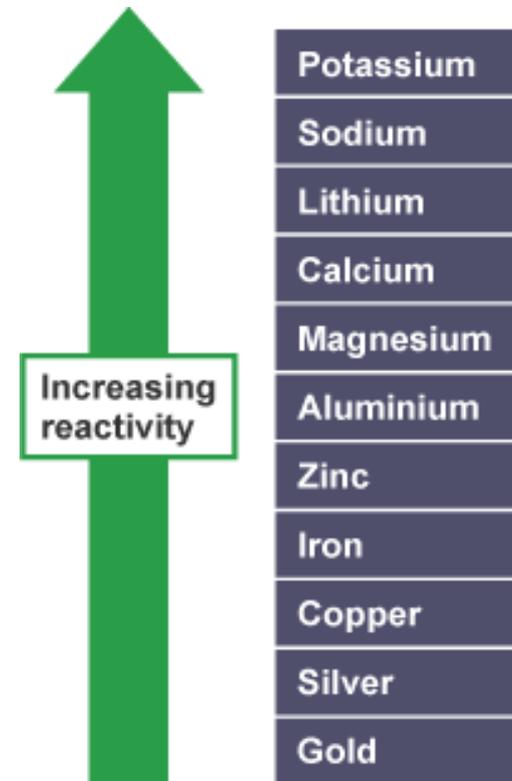
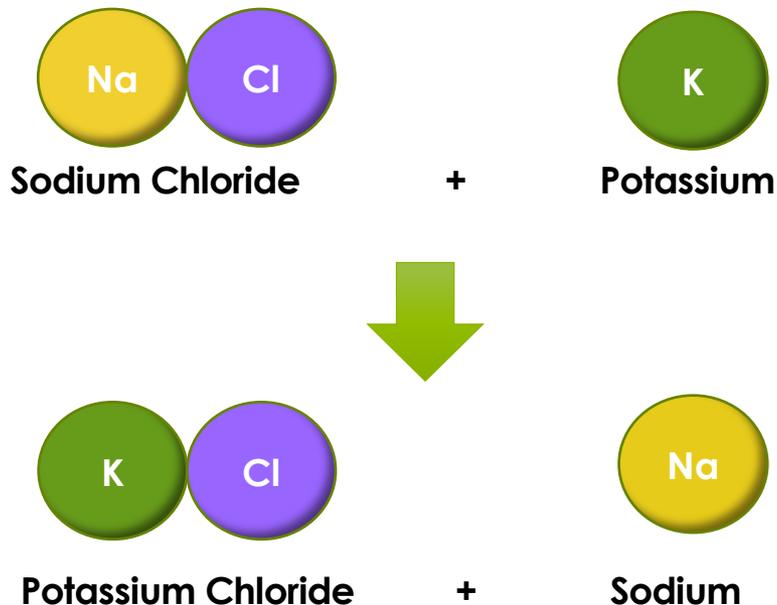
<https://www.youtube.com/watch?v=y0hrqLTubDM>



<https://bam.files.bbc.co.uk/bam/live/content/zb7y4wx/small>

Reactivity Series

If we took normal table salt, **Sodium Chloride**, and introduced **Potassium** to it:

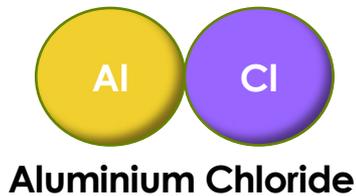


<https://bam.files.bbc.co.uk/bam/live/content/zb7y4wx/small>

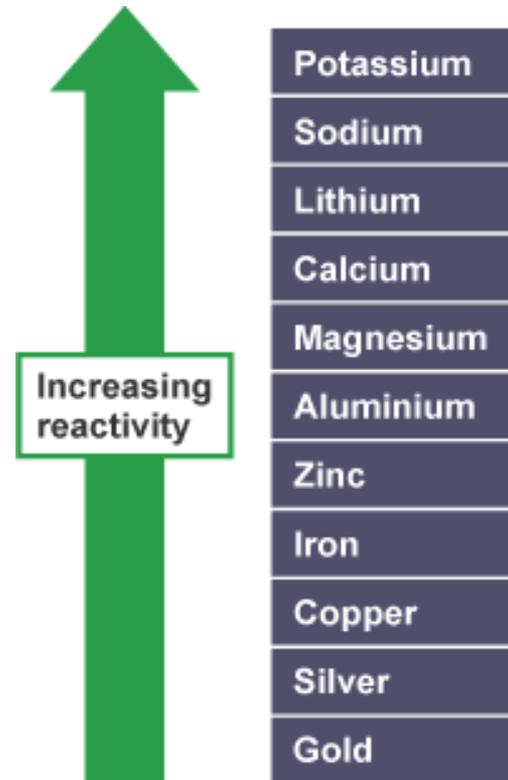
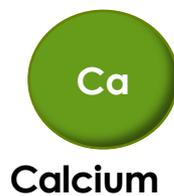
Would a Reaction Occur?

If we have, **Chloride**, and **Calcium** to it:

Aluminium introduced



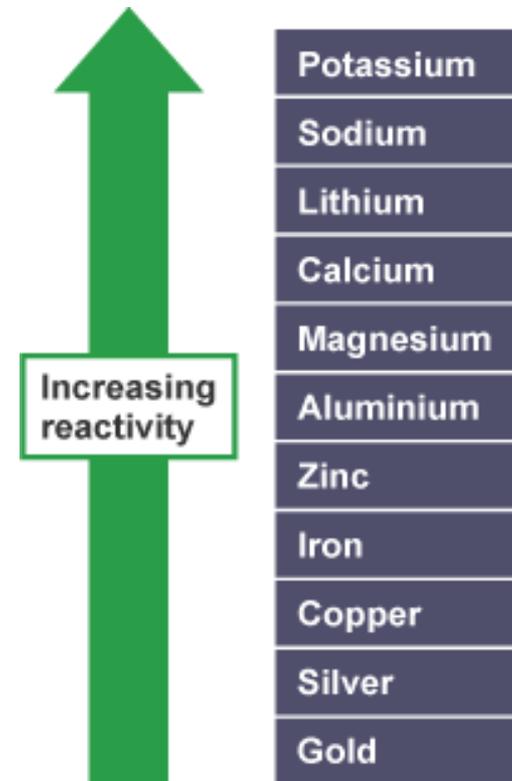
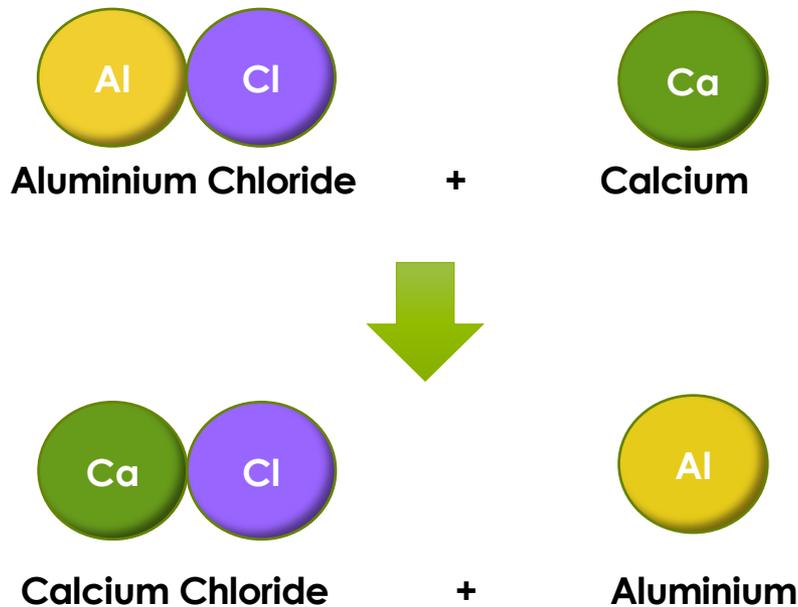
+



Would a Reaction Occur?

If we have, **Chloride**, and **Calcium** to it:

Aluminium introduced

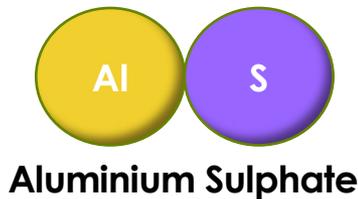


<https://bam.files.bbc.co.uk/bam/live/content/zb7y4wx/small>

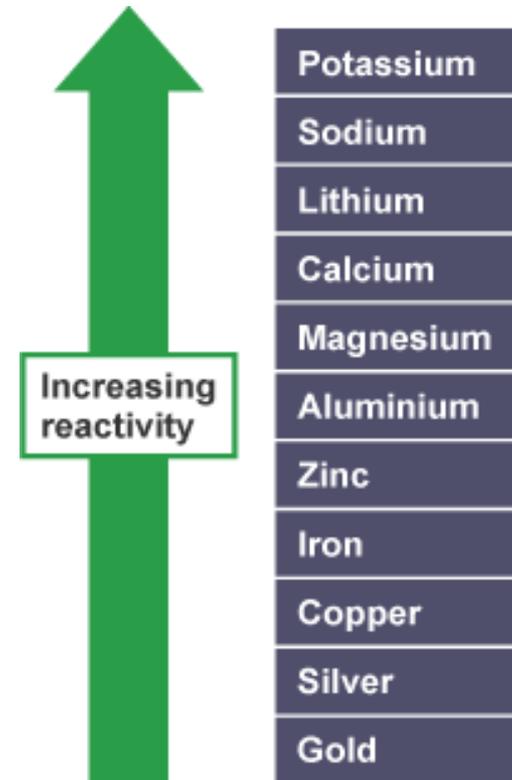
Would a Reaction Occur?

If we have, **Sulphate**, and **Copper** to it:

Aluminium introduced

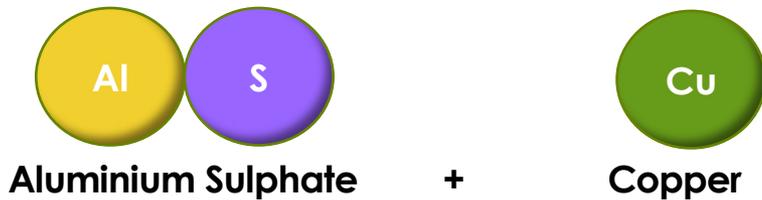


+

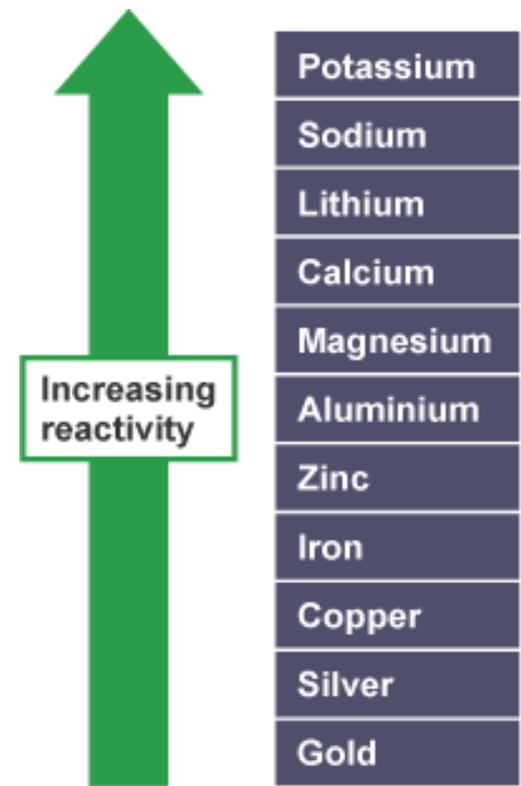


Would a Reaction Occur?

If we have, **Sulphate**, and **Copper** to it: **Aluminium** introduced



No Reaction!



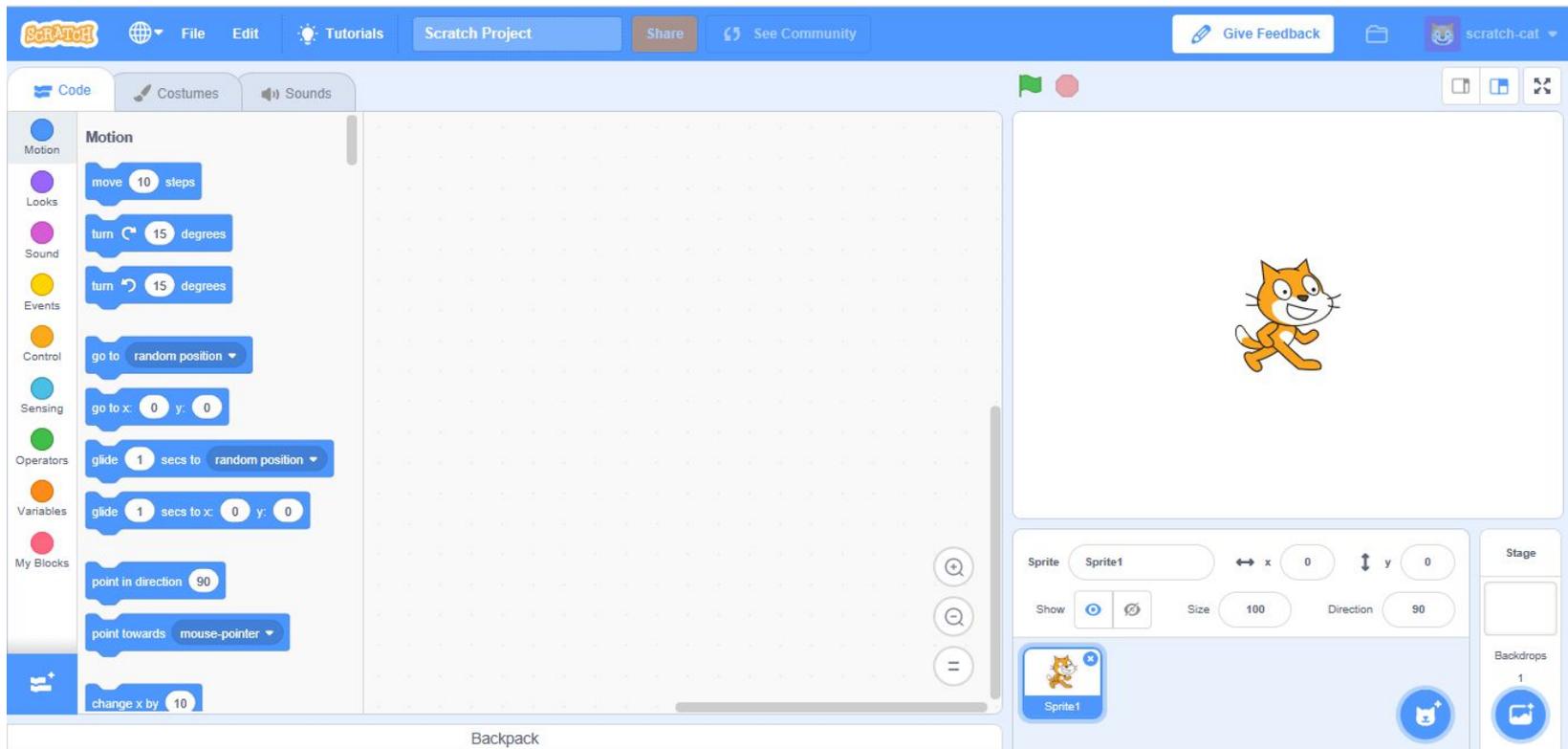
Activity: Complete the Equations

Finish the following equations in your workbooks either by writing the products of the reaction, or writing "No Reaction" if one will not occur.



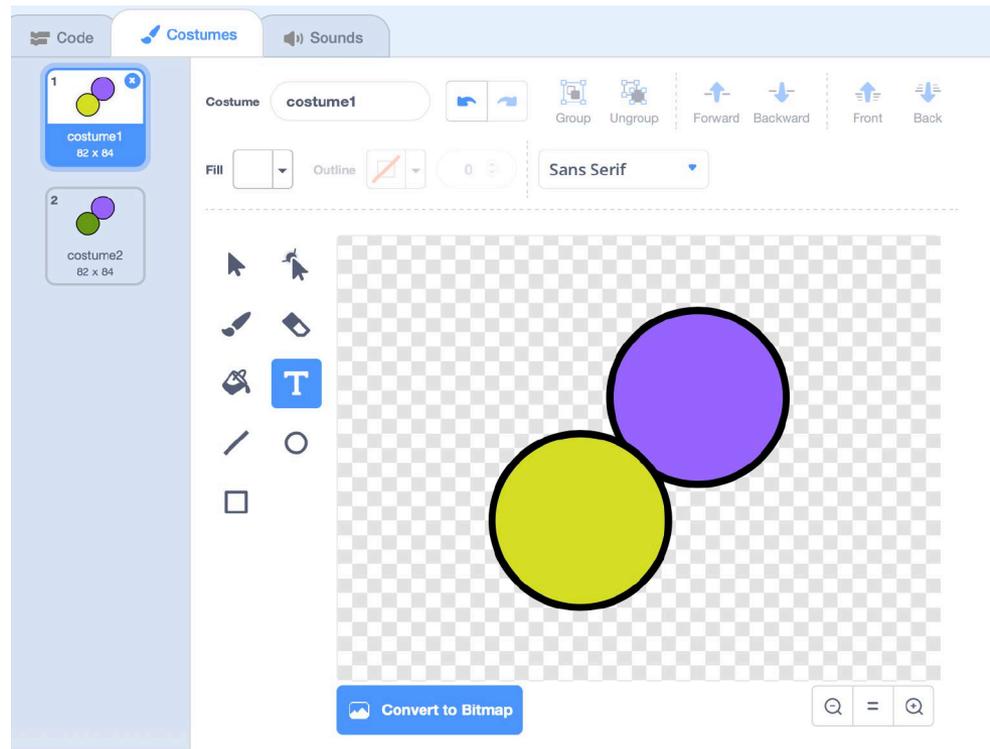
Scratch – Displacement Reaction Simulation

We will now create a Scratch program to simulate a displacement reaction.



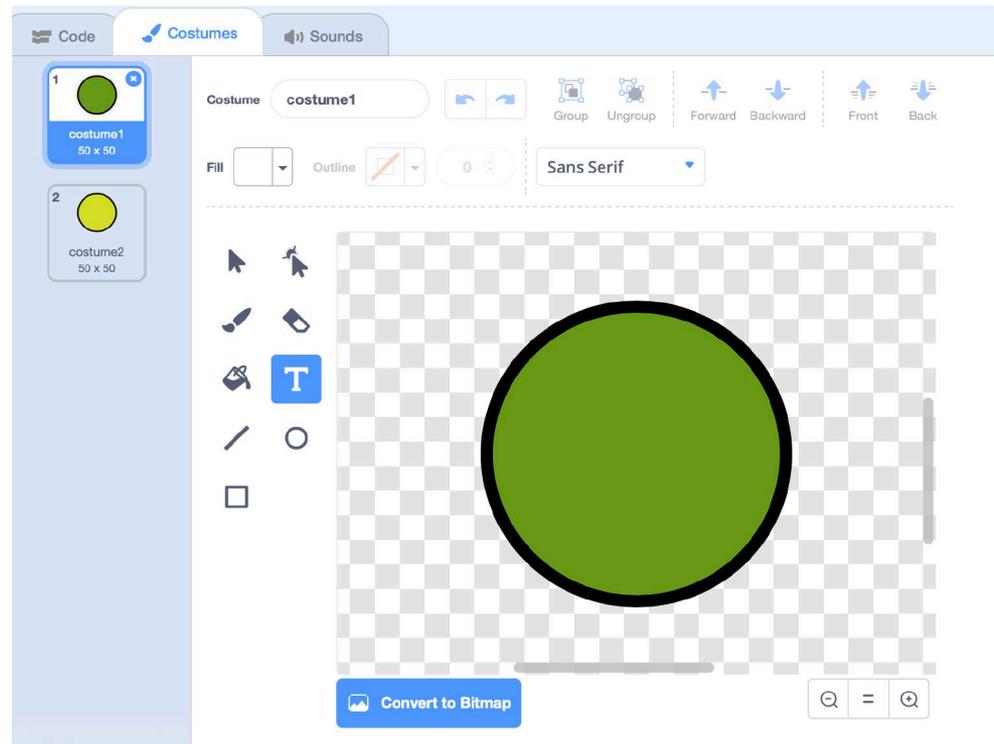
Activity: Designing Our Compound

Design a costume for our compound, a purple and yellow circle together. Add another costume, this time with a purple and green circle.



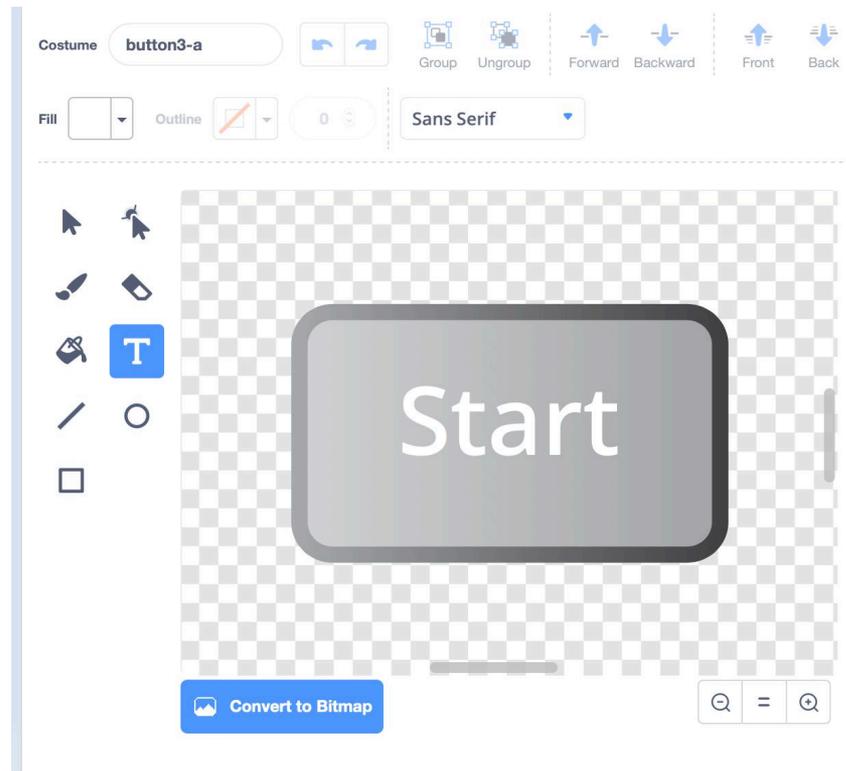
Activity: Designing Our Metal Ion

Design costumes for our Metal ion, one a green circle, and another costume a yellow one.

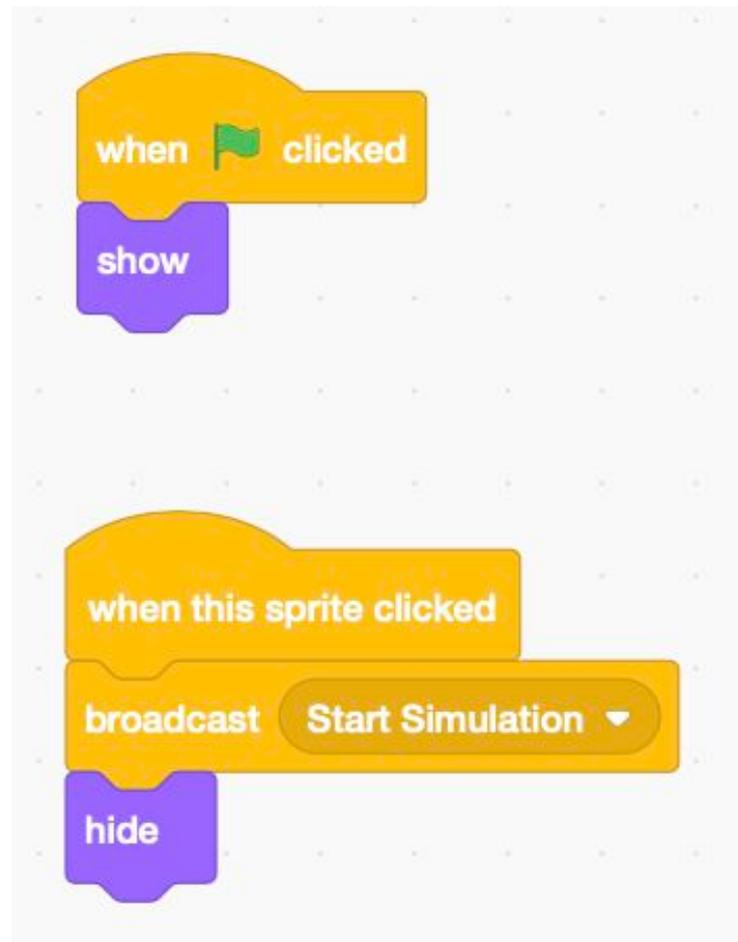


Activity: Designing Our Start Button

Design a start button and program it to broadcast a message when it is clicked.



Button Code



Activity: Coding The Compound

When the game is started the compound should:

1. Switch costume to costume1
2. Go to a specific point on the screen
3. Show.

When the Start button is pressed:

1. Go to a random position
2. Repeatedly move 1 step and then turn a random amount between -10 and 10 degrees.
3. If it touches the Metal ion, switch costume to costume2
4. If it touches the edge, it bounces back in some way.

Compound Code

```

when clicked
  switch costume to costume1
  go to x: -140 y: 0
  show
  
```

```

when I receive Start Simulation
  switch costume to costume1
  go to random position
  repeat 5
    create clone of myself
  forever
    move 1 steps
    turn pick random -10 to 10 degrees
    if touching Metal ? then
      switch costume to costume2
    if on edge, bounce
  
```

Activity: Coding the Metal

When the game is started the compound should:

1. Switch costume to costume1
2. Go to a specific point on the screen
3. Show

When the Start button is pressed:

1. Go to a random position
2. Repeatedly move 1 step and then turn a random amount between -10 and 10 degrees.
3. If it touches the compound, switch costume to costume2
4. If it touches the edge, it bounces back in some way.

Metal Code

```

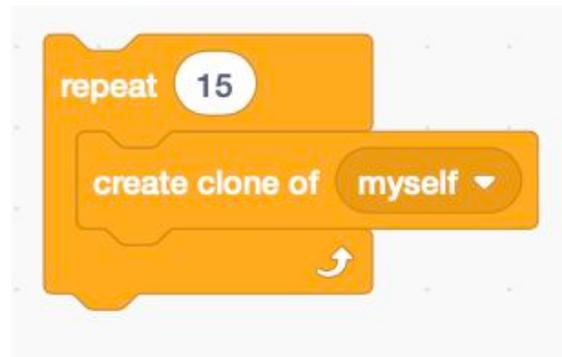
when clicked
  switch costume to costume1
  go to x: 140 y: 0
  show
  
```

```

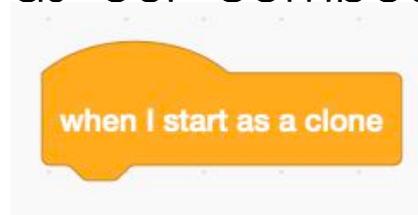
when I receive Start Simulation
  switch costume to costume1
  go to random position
  repeat 5
    create clone of myself
  forever
    move 1 steps
    turn pick random -10 to 10 degrees
    if touching Compound ? then
      switch costume to costume2
    if on edge, bounce
  
```

Activity: Adding More Particles

To add more compound and metal particles, we can use cloning.



These will need to be **placed before the forever loop in our compounds and Metal sprites**. After creating the clones, we will need to tell them how to behave. We want them to behave in exactly the same way as our compound and metal particles already do.



Activity: Edit the Background to Display What is Reacting

Edit the Background by writing in the name of a Compound and Metal which takes part in a displacement reaction.

Activity: Simulating an Experiment

Try to create a scratch program that simulates the following experiment. Think about the molecules and how they change behaviour as temperature changes.

Are there molecules coming off the flame?

