Teacher guide: chemical bonding simulation

Quick reference

The simulation builds ionic and covalent bonds atom by atom with the shell model, and uses experiments to explain the properties of metals and crystals. Its main use is in ESO 4 (Year 11 in the UK, 10th grade in the US), with applications in ESO 3 and Bachillerato 1.

Item	Details
Link	simulaciencia.es/en/simulations/enlaces-quimicos/
Year groups	ESO 4 (main use), ESO 3, Bachillerato 1; occasional review in Bachillerato 2 Chemistry
Subject	Physics and Chemistry; Chemistry in Bachillerato 2
Suggested time	15–20 minutes per type of bond with the simulation projected
Equipment	Projector or interactive whiteboard; runs in the browser, also on phones and tablets, with nothing to install. On narrow screens the canvas moves to the top and the controls below; on a phone the atoms look small, so a large screen is better for explaining
Prior knowledge	Atomic number, arrangement of electrons in shells, metals and non-metals, electric charge
Accessibility	Dark theme only, with no theme or contrast selector. “Pause” button to freeze the animation

How the simulation works

The drop-down at the top of the sidebar chooses the mode: “Ionic Bonding”, “Covalent Bonding” or “Metallic Bonding”. The first two have three slots, “Atom A”, “Atom B” and “Atom C”, each with a selector and a status panel below the canvas. From these two modes you enter a crystal view with the corresponding button and come back with “← Back to bond”.

Mode	What the teacher controls	What it shows
Ionic Bonding	The element in each slot (H, C, N, O, F, Li, Na, Mg, S, Cl, K, Ca or “— Empty —”) and the buttons “Give an electron to B”, “Give an electron to A” and “Give an electron to C”	Atoms with their shells, the charge on each, “Valence e^-: 7 / 8”, whether it reaches an octet or a duet and whether there is attraction with its neighbour. When the bond forms, the “Bond formed” card gives the formula and the ions
Ionic crystal lattice (“View crystal lattice →”)	“3D unit cell” or “2D layer” view. In the layer: “Apply voltage”, “Applied sideways force” from 0 to 150 % of the strength, “Restore the crystal” and the “Forces between the two blocks” and “Show electrons” checkboxes	The real lattice of the compound, the ratio of ions, the surroundings of each ion, that it does not conduct when solid and how it fractures
Covalent Bonding	Non-metals only (H, C, N, O, F, S, Cl). Between neighbouring slots, the “Share”, “Dative” and “Undo” buttons	“Effective e^-: 2 / 2”, “Bonds formed” and the shared pair rotating in the region where the shells overlap
Covalent crystals (“View covalent crystals”)	Crystal: “Diamond”, “Graphite”, “Silica” or “Dry ice”. “Apply voltage” and “Temperature” from −200 to 4000 °C	3D network, type of crystal, properties, vibration of the particles, change of state and conduction (graphite only)

Mode	What the teacher controls	What it shows
Metallic Bonding	"Metal": Na, K, Mg, Ca or Al. "Apply voltage" and "Deform lattice"	A lattice of 20 cations in a sea of 20, 40 or 60 electrons, the melting point, conduction and malleability

Four elements support the explanation:

- **The electron counters.** Each slot shows the charge and the count for the outer shell, for example "Valence e^-: 8 / 8" and "Octet reached". In covalent mode it also counts the shared electrons.
- **The attraction signal.** Between neighbouring slots, "Electrostatic attraction" appears if the charges are opposite and "No electrostatic attraction" if not. It separates the transfer of electrons from the bond itself.
- **The 3D surroundings.** In the 3D cells you rotate by dragging, and clicking an ion or atom highlights its neighbours. Neighbours that lie outside the cell are drawn translucent, so the full coordination number can be seen.
- **The experiments with messages.** Voltage, sideways force, deformation and temperature write what is happening below the lattice, for example "Fracture! — the ionic crystal is brittle".

The "Description" drop-down card summarises each mode and suggests compounds to build: NaCl, $MgCl_2$ and Na_2O in ionic mode; H_2, Cl_2, HCl, H_2O and SO_2 in covalent mode.

Use in each year group

In ESO 3 the simulation is used to introduce the formation of ions and bonding; in ESO 4, to compare the three types of bond and their properties; in Bachillerato 1, for crystals, coordination and dative bonding. It does not fit ESO 2: its curriculum goes as far as the Thomson and Rutherford models. The curriculum content quoted is from the LOMLOE curriculum of the Community of Madrid (Spain), in our own translation.

ESO 3: ions and a first look at bonding

Ages 14–15 · Year 10 in the UK · 9th grade in the US

Curriculum content. Block A: "the laboratory or virtual environments". Block B: "Applying knowledge of the atomic structure of matter to understand the formation of ions", "Atoms and ions" and "Introduction to chemical bonding". Also "writing formulas for and naming elements, monatomic ions and binary compounds".

Objectives. Explain how a cation and an anion form. Relate the charge on an ion to the electrons gained or lost. Distinguish giving electrons from sharing them. Write the formula of simple binary compounds.

Teaching sequence (15–20 min).

1. "Ionic Bonding" mode with the starting set-up: A = Na, B = Cl. Read the panels: Na has "Valence e^-: 1 / 8" and Cl "7 / 8". Ask what is easier for each of them.
2. Press "Give an electron to B". Na changes to "Charge: +" and Cl to "Charge: −", both with 8 / 8. "Electrostatic attraction" appears and the card gives NaCl. Define cation and anion.
3. Set up A = Cl, B = Mg, C = Cl. The Mg panel says "Still needs to lose 2 e^-". Press "Give an electron to A" and "Give an electron to C". The result is Mg^{2+} with two Cl^- and the formula $MgCl_2$: 12 protons and 10 electrons give a 2+ charge.

4. Switch to “Covalent Bonding”: the starting set-up is H and H, each with “Effective e⁻: 1 / 2”. Press “Share”: both reach 2 / 2 and the card gives H_2.
5. Set up A = H, B = O, C = H. O starts at 6 / 8. Press “Share” between A and B and between B and C: O reaches 8 / 8 and H_2O appears. Stress that no atom is left with a charge.

ESO 4: the three types of bond and their properties

Ages 15–16 · Year 11 in the UK · 10th grade in the US

Curriculum content. Block A: “the laboratory or virtual environments”. Block B: “Electron configuration of the elements and position in the periodic table”, “Chemical bonding: ionic, covalent and metallic” and “Chemical compounds of particular interest”.

Objectives. Explain ionic, covalent and metallic bonding with the shell model. Recognise that ionic compounds form lattices, not molecules. Justify conductivity, brittleness and malleability in terms of structure. Distinguish covalent networks from molecular substances.

Teaching sequence (15–20 min).

1. “Ionic Bonding” with Na and Cl, press “Give an electron to B” and then “View crystal lattice →”. In “3D unit cell” the card says “Sodium chloride type”. Click a Na^+: its 6 Cl^- are highlighted. There are no NaCl molecules.
2. Switch to “2D layer” and press “Apply voltage”: “Does not conduct when solid — ions fixed in the lattice”. Remove the voltage and take “Applied sideways force” to 80 %: “Elastic deformation”. Raise it to 120 %: the layers slide and “Fracture! — the ionic crystal is brittle” appears.
3. Go back with “Restore the crystal”, tick “Forces between the two blocks” and move the force again. As the layers slide, red repulsion arrows appear between ions with the same charge.
4. “Metallic Bonding” mode with Na: “e^- in the sea: 20”. Press “Apply voltage”: the electrons move towards the + terminal and “Electrical conductivity” appears. Press “Deform lattice”: “The bond does not break — malleability”. Compare it with the fracture in step 2.
5. “Covalent Bonding” mode, “View covalent crystals” button. In “Diamond”, raise the temperature to about 2000 °C: it is still solid, because it melts at 3550 °C. In “Dry ice”, go from −100 °C to −75 °C: “Sublimes at −78 °C! The molecules separate whole”.
6. Press “Apply voltage” in “Diamond” and in “Graphite”. Diamond does not conduct; graphite does, because the fourth electron of each C moves through the sheet.

Bachillerato 1: crystals, coordination and dative bonding

Ages 16–17 · Year 12 in the UK · 11th grade in the US

Curriculum content. Block A: “The covalent bond: Lewis structures for covalent bonding”, “Intermolecular forces” and “Structure and properties of substances with covalent bonding: molecular substances and covalent networks”. Also “The ionic bond. Ionic crystals. Properties of ionic compounds” and “The metallic bond. Structure and properties”.

Objectives. Relate the ratio of ions to the structure and the coordination number. Build single, double, triple and dative bonds using the Lewis criterion. Compare covalent networks, molecular crystals and metallic lattices.

Teaching sequence (15–20 min).

1. In “Ionic Bonding”, set up A = Na, B = O, C = Na and give one electron from each Na to the O. In the lattice, the card says “Antifluorite type”, “2 Na^+ for every O^{2-}” and “$2\cdot(+1) + 1\cdot(-2) = 0$ → neutral

crystal". Each Na^+ has 4 O^{2-} and each O^{2-} has 8 Na^+.

2. Repeat with A = F, B = Ca, C = F: "Fluorite type", with coordination 8 for Ca^{2+} and 4 for F^-. Compare with the 6:6 of NaCl and ask why it changes.
3. Set up $MgCl_2$ (A = Cl, B = Mg, C = Cl): "Cadmium chloride type (layered)". In "2D layer", with the force at 120 %, the sheets slide without breaking. Compare with MgO (A = Mg, B = O, "Give an electron to B" twice), which fractures.
4. In "Covalent Bonding", set up A = N, B = N and press "Share" three times: 8 / 8 and "Bonds formed: 3". Relate it to the Lewis structure of N_2.
5. Build SO_2 (A = O, B = S, C = O): "Share" twice between A and B and "Dative" once between B and C. The lens of the dative bond takes on the colour of S and carries an S→O arrow.
6. In "View covalent crystals", choose "Silica": "Each Si is bonded to 4 O" and "SiO_2 gives the ratio of atoms". Take it above 1713 °C: "Covalent bonds break". Contrast it with dry ice, where only intermolecular forces are overcome.

Bachillerato 2 Chemistry: occasional review

Ages 17–18 · Year 13 in the UK · 12th grade in the US

The simulation does not calculate energies, so it cannot be used for the "Born-Haber cycle". It can serve as a visual review of the "characteristics of covalent and molecular solids" with the four covalent crystals. It also illustrates the "electron cloud model" of a metal, though not band theory. It is best used alongside VSEPR theory, because it draws every molecule in a line.

Misconceptions it helps to address

The simulation mainly tackles two ideas: that the bond is the transferred electron, and that everything is made of molecules. Each row gives a common prior idea and how to break it down with the simulation.

Students' idea	Correct idea	How to show it
"The ionic bond is the electron that moves from the metal to the non-metal"	The transfer forms the ions; the bond is the electrostatic attraction between them	Na and Cl before the transfer: "No electrostatic attraction". After "Give an electron to B": "Electrostatic attraction" and "Ionic bond · Coulomb attraction"
"Salt is made of NaCl molecules"	It is a lattice of ions with no molecules; the formula gives the ratio	"View crystal lattice →", "3D unit cell", click a Na^+: it has 6 Cl^- neighbours, all at the same distance
"Each Na^+ is only bonded to the Cl^- that received its electron"	Each ion attracts all its neighbours of opposite charge	In the same cell, click a Cl^-: it also has 6 Na^+. With "Show electrons" in the 2D layer, all the Cl^- ions are identical
"Ionic compounds conduct because they have ions"	When solid they do not conduct: the ions cannot move	"2D layer", "Apply voltage": "Does not conduct when solid — ions fixed in the lattice"
"All covalent substances melt at low temperatures"	Covalent networks have extremely high melting points	"Diamond" at about 2000 °C is still solid; "Dry ice" sublimes at −78 °C
"When dry ice sublimes, the CO_2 molecules break up"	Whole molecules separate; only the intermolecular forces are overcome	"Dry ice" from −100 °C to −75 °C: "No covalent bond breaks: only the weak forces between molecules"

Students' idea	Correct idea	How to show it
“In a metal the electrons only move when there is a current”	They always move at random; the voltage adds a net drift towards the + terminal	“Metallic Bonding” in “Normal (equilibrium)”: electrons in all directions. With “Apply voltage” they drift together towards +
“If it is carbon, graphite and diamond behave the same”	The structure determines the properties	“Apply voltage” in “Diamond” (“Does not conduct electricity”) and in “Graphite” (“Conducts: electrons move along the sheets”)

Simplifications worth knowing

The simulation puts counting electrons and relating structure to properties first. To do so it simplifies the atoms, the geometries and the energies. It is worth knowing about these liberties so as not to reinforce wrong ideas by accident.

1. **Bohr atoms with fixed shells.** The shells always have radii of 36, 60, 84 and 108 pixels and the nucleus is the same size in every element. The size does not reflect the atomic radius. K is drawn as 2, 8, 8, 1, with no subshells. In Bachillerato 1 it is worth reminding students that orbitals replace these orbits.
2. **The octet decides everything.** An atom is stable if its outer shell has 8 electrons, or 2 for H and Li. There are no ionisation energies, electron affinity or lattice energy. Also, the teacher can give electrons in either direction and keep giving after the octet: the panel then shows “1 e^- too many” on the non-metal or, if a metal has given too many (Na^{2+}), “Lost too many: must take back 1 e^-”. In Bachillerato 2 it has to be explained that the crystal is stable because of the lattice energy.
3. **At most three atoms in a line.** The slots only give or share with their neighbour, so the compounds formed are MX, M_2X or MX_2. Li_3N, CH_4 or NH_3 cannot be built, and Al only appears in metallic mode. The green box of “Ionic bond formed!” groups the ions as if they were a molecule: add this nuance before moving on to the lattice.
4. **All molecules are linear.** H_2O and SO_2 appear with the three atoms in a line, when they are bent. “Bonds formed” counts pairs: a double bond adds 2. SO_2 with a dative bond is the classic Lewis model; today it is described with resonance.
5. **Ball-and-stick ionic lattices.** The distances come from Shannon ionic radii: for NaCl, the cell edge is 2·(1.02 + 1.81) = 5.66 Å, compared with the real 5.64 Å. The spheres are drawn at 55 % of the ionic radius so the inside can be seen, so the lattice looks hollow. CaH_2 is shown as fluorite as an approximation and the 2D layer of $CaCl_2$ as undistorted rutile.
6. **Sideways force as a percentage.** The slider does not give newtons: 100 % is the maximum force that interface can resist according to the model (Coulomb, Born repulsion with exponent 9 and van der Waals). If you jump suddenly to almost 100 %, some lattices such as Na_2O or CaF_2 already break because of inertia. In $MgCl_2$, only van der Waals forces and repulsion are calculated between the sheets.
7. **A toy metal.** The lattice has 5 × 4 = 20 cations and each one contributes its valency to the sea: 20 electrons with Na or K, 40 with Mg or Ca and 60 with Al. The electrons do not collide with the ions and their drift under a voltage is hugely exaggerated. When deformed, the top two rows slide a whole lattice period at once, dragging their part of the electron sea with them, with no dislocations: in a real metal slip happens gradually.
8. **Temperature with a simple criterion.** The vibration follows the Lindemann criterion: the amplitude is 10 % of the distance between neighbours multiplied by √(T / T of change), in kelvin. The change of state

happens all at once at a fixed temperature: 3550 °C for diamond, 3650 °C for graphite, 1713 °C for silica and −78 °C for dry ice. There is no pressure and no latent heat.

9. **Idealised silica.** Cristobalite is shown with straight Si–O–Si bonds and an Si–O distance of 1.55 Å, a little shorter than the real one. The card itself notes that quartz, which is more common, has the same SiO_4 tetrahedra.

Student activity worksheet

The activity worksheet follows a predict, observe and explain structure. Each activity links to the simulation already set up, so it works in the computer room, with tablets or as homework. It downloads in Word and LibreOffice formats so it can be adapted.

Year group	Activities	Suggested time
ESO 3 (Year 10)	Before you start (a, b and c), activities 1, 2 and 4, problems 1, 2 and 4 of Apply what you have learnt and Self-assessment	One 50–55 minute lesson
ESO 4 (Year 11)	The whole worksheet except Going further	Two lessons, or one if activities 1 and 2 are set as homework
Bachillerato 1 (Year 12)	Activities 3, 5 and 6, Going further and problem 3 of Apply what you have learnt	One lesson

The “Before you start” table collects six prior ideas about bonding. It is best not to correct it at the beginning: students come back to it in “Review your ideas”. In activity 4 the simulation draws all the molecules in a line; if geometry is being taught, point out that H_2O is bent.

Answers

Section	Answer
Before you start	All false. a) The transfer forms the ions; the bond is the electrostatic attraction between them (activity 1). b) It is a lattice of ions; the formula gives the ratio (activity 3). c) In the solid the ions are fixed and do not conduct (activity 3). d) Covalent networks, such as diamond, melt at extremely high temperatures (activity 6). e) They always move randomly; the voltage adds a drift towards the + terminal (activity 5). f) Structure decides the properties: graphite conducts and diamond does not (activity 6)
Activity 1	Before: Na with charge 0 and “Valence e^-: 1 / 8”; Cl with charge 0 and “7 / 8”; “No electrostatic attraction”. After: Na with charge + and 8 / 8; Cl with charge − and 8 / 8; “⚡ Electrostatic attraction”. It is easier for Na to lose 1 electron than to gain 7. Na^+ is the cation (positive ion) and Cl^- the anion (negative ion). They are held together by the attraction between opposite charges, not by the transferred electron
Activity 2	Cl, Mg, Cl: Mg gives 2 e^-, one to each Cl; ions Mg^{2+} and 2 Cl^-; $MgCl_2$. Na, O, Na: each Na gives 1 e^- to O; ions 2 Na^+ and O^{2-}; Na_2O. Ca, O: Ca gives 2 e^- to O; ions Ca^{2+} and O^{2-}; CaO. Each Cl only accepts 1 electron and Mg must give 2; O needs 2 and each Na gives only 1. The charges always add up to 0: the compound is neutral
Activity 3	Each Na^+ has 6 Cl^- neighbours and each Cl^- has 6 Na^+. Voltage: “Does not conduct when solid — ions fixed in the lattice”. 80 %: “Elastic deformation”. 120 %: the layers slide and you get “Fracture! — the ionic crystal is brittle”. There are no molecules: the formula NaCl means there is one Na^+ for each Cl^-. It does not conduct because the ions cannot move. When a layer slides, ions of the same charge end up facing each other, they repel (red arrows) and the crystal splits
Activity 4	Two non-metals both tend to gain electrons; neither gives them away, so they share them. H, H: 1 / 2 each, 1 press, 1 bond, H_2. H, O, H: H 1 / 2 and O 6 / 8, 2 presses (A–B and B–C), O with “Bonds formed: 2”, H_2O. N, N: 5 / 8 each, 3 presses, 3 bonds, N_2. No atom is left with a charge: the electrons are shared instead of moving from one atom to the other. N has 5 valence electrons and needs 3 more: it forms a triple bond

Section	Answer
Activity 5	Na: 1 valence e^-, 20 e^- in the sea, 98 °C. Mg: 2, 40, 650 °C. Al: 3, 60, 660 °C. With no voltage the electrons move randomly in all directions; with voltage they drift towards the + terminal (“Electrical conductivity”); when deformed, the layers slide and the bond does not break (“malleability”). Metals conduct because their electrons move freely through the lattice. When the layers slide, the cations are still surrounded by the sea of electrons; in the ionic crystal, like charges face each other. The more electrons in the sea, the stronger the bond and usually the higher the melting point (Al is the exception in the table: it melts at 660 °C, almost the same as Mg)
Activity 6	Diamond: covalent crystal, C atoms, melts at 3550 °C, does not conduct. Graphite: layered covalent crystal, C atoms in sheets, sublimes at 3650 °C, conducts along the sheets. Dry ice: molecular crystal, CO_2 molecules, sublimes at −78 °C, does not conduct. When it sublimes no C=O bond is broken: only the weak forces between molecules are overcome. Diamond is a network of covalent bonds: to melt it, many of them must be broken. In graphite each C uses 3 electrons in bonds and the fourth is free to move along the sheet
Apply what you have learnt	1) K: 2, 8, 8, 1 → K^+. S: 2, 8, 6 → S^{2-}. K_2S. 2) KCl ionic; Cl_2 covalent; Cu metallic; CO_2 covalent (molecular); CaO ionic. 3) Ionic (it is NaCl): when dissolved, the ions are free to move. 4) H–Cl, one shared pair; O=O, two shared pairs (double bond)
Going further	1) Antifluorite structure: each Na^+ has 4 O^{2-} and each O^{2-} has 8 Na^+; as there are twice as many Na^+ as O^{2-}, the coordination of O^{2-} is double. 2) In the dative bond both electrons of the pair come from one atom, here S (arrow S→O). 3) Silica is a covalent network: above 1713 °C covalent Si–O bonds break; in dry ice only intermolecular forces were overcome

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