

Two Atoms Screen

Change the electronegativity of the atoms, view the resulting electrostatic potential or electron density, and predict the bond polarity.

The screenshot shows the 'Two Atoms' screen in the PhET Molecule Polarity simulation. At the top, a color scale for 'Electrostatic Potential' ranges from positive (blue) to negative (red). The central diagram shows two atoms, A (yellow) and B (green), with partial charges δ^- and δ^+ respectively, and a dipole arrow pointing from A to B. Below the atoms are two electronegativity sliders for Atom A and Atom B, each with a scale from 'less' to 'more'. A 'Bond Character' slider at the bottom indicates the range from 'more covalent' to 'more ionic'. On the right, a 'View' panel includes checkboxes for 'Bond Dipole', 'Partial Charges', and 'Bond Character', and radio buttons for 'Surface' (None, Electrostatic Potential, Electron Density). An 'Electric Field' toggle is also present. A navigation bar at the bottom includes 'Molecule Polarity', 'Two Atoms', 'Three Atoms', 'Real Molecules', and the PhET logo.

VIEW partial charges

DETERMINE if the bond is more covalent or more ionic

ADJUST the electronegativity

EXPLORE different surfaces

REVERSE the convention for the direction of dipole moment

Three Atoms Screen

Explore the relationship between the bond dipoles and the molecular dipole, and observe the molecule in an electric field.

The screenshot shows the 'Three Atoms' screen in the PhET Molecule Polarity simulation. The central diagram shows three atoms: A (yellow), B (green), and C (pink), arranged in a bent shape. Bond dipoles are shown as arrows pointing from each atom towards the center. A molecular dipole arrow is shown pointing from the center towards the right. The molecule is placed between two vertical plates representing an electric field, with a negative plate on the left and a positive plate on the right. Below the atoms are three electronegativity sliders for Atom A, Atom B, and Atom C, each with a scale from 'less' to 'more'. On the right, a 'View' panel includes checkboxes for 'Bond Dipoles', 'Molecular Dipole', and 'Partial Charges', and an 'Electric Field' toggle (currently on). A navigation bar at the bottom includes 'Molecule Polarity', 'Two Atoms', 'Three Atoms', 'Real Molecules', and the PhET logo.

DRAG atoms A or C to adjust the bond angle

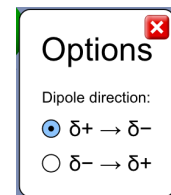
DRAG atom B to rotate

RELATE the bond dipoles to the molecular dipole

OBSERVE the atoms in an Electric Field

Complex Controls

- The direction for the bond dipole points from partial positive to partial negative, by default. The direction can be reversed by opening the PhET menu, selecting Options, and choosing the desired convention.

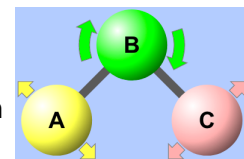


Model Simplifications

- The electronegativity slider ranges from 2 to 4, but the value is never displayed. The resulting electronegativity difference between two bonded atoms varies from 0 to 2.
- Bond dipoles are parallel to the bond axis, and their length is linearly proportional to the difference in electronegativity. Note that this is a simplification; in reality, the dipole is not influenced solely by electronegativity.
- The molecular dipole is the vector sum of the bond dipoles. In the Two Atoms screen, the molecular dipole is not shown, as it is equivalent to the bond dipole. In the Three Atoms screen, manipulating electronegativity results in an understanding of summing vector magnitudes, while manipulating bond angles results in an understanding of summing vector angles.
- The magnitude of an atom's partial charge is linearly proportional to the electronegativity difference between the bonded pair. If an atom has a higher electronegativity than the atom at the other end of the bond, then the partial charge's sign is negative; otherwise it is positive. For atoms that participate in more than one bond (e.g., atom B in the "Three Atoms" screen), net partial charge is the sum of the partial charges contributed by each bond.
- The electrostatic potential and electron density are linearly proportional to the electronegativity difference set by the sliders. These surfaces are not implemented for the triatomic molecule in the Three Atoms screen, because the manipulation of bond angles results in undefinable surfaces.
- The Three Atoms screen allows for students to change the bond angle between the outer atoms (A & C). The AB and BC bonds are treated independently, and the model does not allow for these atoms to repel each other. To explore how atoms would repel one another when the bond angles are changed, see the [Molecule Shapes](#) simulation. The AB and BC bonds are treated independently.
- The Real Molecules screen is not currently available in HTML5. If your device runs Java, you can use the [Java version](#) of the sim.

Insights Into Student Use

- In interviews, no students thought that you can change the electronegativity of a **real** atom.
- Students can rotate the molecule in 2D and change the bond angle (Three Atoms screen). In initial interviews, many students did not find this control, so arrows were added. These arrows will be dismissed once a student interacts with the molecules.



Suggestions for Use

Sample Challenge Prompts

- Predict how changing electronegativity will affect the bond polarity.
- Explain the relationship between the bond dipoles and the molecular dipole.
- Determine if a non-polar molecule can contain polar bonds.
- Describe how the ABC bond angle effects the molecular dipole.
- Compare the behavior of non-polar and polar molecules in an external electric field.

See all published activities for Molecule Polarity [here](#).

For more tips on using PhET sims with your students, see [Tips for Using PhET](#).