

### 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. It features a central diatomic molecule with two atoms, A and B, connected by a bond. Atom A is yellow and labeled with a partial negative charge ( $\delta^-$ ), while Atom B is green and labeled with a partial positive charge ( $\delta^+$ ). A double-headed arrow above the bond indicates the bond dipole. The background is color-coded by electrostatic potential, with red representing positive and blue representing negative. Below the molecule are two sliders for 'Atom A Electronegativity' and 'Atom B Electronegativity', each with a scale from 'less' to 'more'. A 'Bond Character' slider is positioned above these, ranging from 'more covalent' to 'more ionic'. To the right is a 'View' control panel with checkboxes for 'Bond Dipole', 'Partial Charges', and 'Bond Character', and radio buttons for 'Surface' (None, Electrostatic Potential, Electron Density). Below the surface controls is an 'Electric Field' toggle switch. 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. It features a triatomic molecule with three atoms: A (yellow), B (green), and C (pink). Atoms A and C are positioned above and below atom B, respectively. Each atom has a partial charge label ( $\delta^-$  for A,  $\delta^+$  for B, and  $\delta^-$  for C). Bond dipoles are shown as arrows pointing from each atom towards the other. A larger arrow represents the molecular dipole. The molecule is placed between two vertical grey plates representing an electric field, with a negative sign on the left and a positive sign on the right. Below the molecule are three sliders for 'Atom A Electronegativity', 'Atom B Electronegativity', and 'Atom C Electronegativity'. To the right is a 'View' control panel with checkboxes for 'Bond Dipoles', 'Molecular Dipole', and 'Partial Charges', and an 'Electric Field' toggle switch. 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

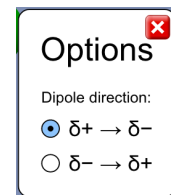
**DRAG** atom B to rotate

**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.

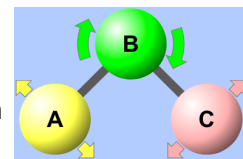


## Model Simplifications

- 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](#).