

## 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 model of two atoms, A (yellow) and B (green), connected by a bond. Atom A has a partial negative charge ( $\delta^-$ ) and Atom B has a partial positive charge ( $\delta^+$ ). A color-coded electrostatic potential map surrounds the atoms, with red indicating negative potential and blue indicating positive potential. Below the atoms are two sliders for 'Electronegativity' for Atom A and Atom B, ranging from 'less' to 'more'. A 'Bond Character' indicator shows a scale from 'more covalent' to 'more ionic'. On the right, a control panel includes a 'View' section with checkboxes for 'Bond Dipole', 'Partial Charges', and 'Bond Character'. Below this is a 'Surface' section with radio buttons for 'None', 'Electrostatic Potential' (selected), and 'Electron Density'. At the bottom of the control panel is an 'Electric Field' section with a toggle switch set to 'off'. Callout boxes provide instructions: 'VIEW partial charges' points to the partial charges; 'DETERMINE if bonds are more ionic or covalent' points to the Bond Character indicator; 'ADJUST the electronegativity' points to the electronegativity sliders; 'EXPLORE different surfaces' points to the Surface selection; and 'REVERSE convention for dipole moment direction' points to the Bond Dipole checkbox. The bottom of the screen shows a navigation bar with icons for 'Two Atoms', 'Three Atoms', and 'Real Molecules'.

**VIEW** partial charges

**DETERMINE** if bonds are more ionic or covalent

**ADJUST** the electronegativity

**EXPLORE** different surfaces

**REVERSE** convention for dipole moment direction

## 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 central model of three atoms, A (yellow), B (green), and C (pink), arranged in a bent shape. Atom B is the central atom. Each atom has an electronegativity slider. Bond dipoles are shown as arrows pointing from the less electronegative atom to the more electronegative atom. A molecular dipole arrow is shown pointing from the center of the molecule towards the more electronegative side. 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. A control panel on the right includes a 'View' section with checkboxes for 'Bond Dipoles', 'Molecular Dipole', and 'Partial Charges'. Below this is an 'Electric Field' section with a toggle switch set to 'on'. Callout boxes provide instructions: 'ADJUST bond angle with atoms A and C' points to the bond angle; 'ROTATE molecule with atom B' points to the central atom B; 'RELATE the bond dipoles to the molecular dipole' points to the molecular dipole arrow; and 'OBSERVE molecule in an electric field' points to the electric field toggle. The bottom of the screen shows a navigation bar with icons for 'Two Atoms', 'Three Atoms' (selected), and 'Real Molecules'.

**ADJUST** bond angle with atoms A and C

**ROTATE** molecule with atom B

**RELATE** the bond dipoles to the molecular dipole

**OBSERVE** molecule in an electric field

## Customization Options

Query parameters allow for customization of the simulation, and can be added by appending a '?' to the sim URL, and separating each query parameter with an '&'. The general URL pattern is:

```
...html?queryParameter1&queryParameter2&queryParameter3
```

For example, in Molecule Polarity, if you only want to include the 1st and 2nd screens (`screens=1,2`), with the 2nd screen open by default (`initialScreen=2`) use:

[https://phet.colorado.edu/sims/html/molecule-polarity/latest/molecule-polarity\\_all.html?screens=1,2&initialScreen=2](https://phet.colorado.edu/sims/html/molecule-polarity/latest/molecule-polarity_all.html?screens=1,2&initialScreen=2)

To run this in Spanish (`locale=es`), the URL would become:

[https://phet.colorado.edu/sims/html/molecule-polarity/latest/molecule-polarity\\_all.html?locale=es&screens=1,2&initialScreen=2](https://phet.colorado.edu/sims/html/molecule-polarity/latest/molecule-polarity_all.html?locale=es&screens=1,2&initialScreen=2)

⚙ Indicates this customization can be accessed from the Preferences menu within the simulation.

Query Parameter and Description	Example Links
⚙ <code>dipoleDirection</code> - the direction for the bond dipole points from partial positive to partial negative by default ( <code>positiveToNegative</code> ) and can be displayed in the reverse direction ( <code>negativeToPositive</code> ).	<code>dipoleDirection=negativeToPositive</code>
<code>screens</code> - specifies which screens are included in the sim and their order. Each screen should be separated by a comma. For more information, visit the <a href="#">Help Center</a> .	<code>screens=1</code> <code>screens=1,2</code>
<code>initialScreen</code> - opens the sim directly to the specified screen, bypassing the home screen.	<code>initialScreen=1</code> <code>initialScreen=2</code>
⚙ <code>locale</code> - specify the language of the simulation using <a href="#">ISO 639-1</a> codes. Available locales can be found on the simulation page on the <a href="#">Translations tab</a> . Note: this only works if the simulation URL ends in "_all.html".	<code>locale=es</code> (Spanish) <code>locale=fr</code> (French)
<code>allowLinks</code> - when <code>false</code> , disables links that take students to an external URL. Default is <code>true</code> .	<code>allowLinks=false</code>
<code>supportsPanAndZoom</code> - when <code>false</code> , disables panning and zooming using pinch-to-zoom or browser zoom controls. Default is <code>true</code> .	<code>supportsPanAndZoom=false</code>

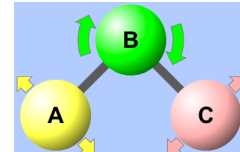
## Model Simplifications

- 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.
- When the electric field is turned on, the molecule's angular velocity is proportional to the molecular dipole moment. If the molecular dipole is tiny (but non-zero) it can rotate over several minutes.
- 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](#).