

## Two Atoms Screen

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

**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.

**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 a '&'. 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`

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`

⊗ 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 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><br><code>screens=1,2</code>                  |
| <code>initialScreen</code> - opens the sim directly to the specified screen, bypassing the home screen.  | <code>initialScreen=1</code><br><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 <code>“_all.html”</code> . | <code>locale=es</code> (Spanish)<br><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>                               |

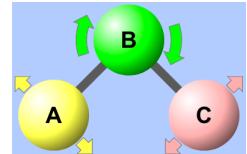
## Model Simplifications

- 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](#).