Molecule Polarity

Other ideas for the title:
Molecular Polarity
Molecules and Polarity
Molecule Polarity (consensus 7/8/11)
Polarity of Molecules
Polarity and Molecules
Polarity and Bonding
Polar Molecules
Polar and Nonpolar Molecules
Chemical Polarity

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Public URL
https://docs.google.com/document/pub?id=1fzKjSF0yGmy9lCJ_zBZvWo3F6FqKpzy-EqaBh1EFyEk

Contents

Learning Goals

From the chem advisory board
“One major shortcoming of the chemistry sims that have been produced to date is the absence of the relationship between structure and properties. One great advantage of technology is

the ability to provide visualizations of molecular level structures – which can be related to the properties. While many of the sims do provide multiple data sources while processes are occurring, it seems that these different data sources (which can be toggled on and off) are usually only different ways of representing the number of particles in solution. We recommend that more attention be given to showing the types of particles present and the way their structures affect their properties and the process being investigated."

Audience
This sim is designed for students in intro-level college chemistry. This concept is often taught after VSEPR theory. Students need to be able to predict the molecular shape correctly before they can predict molecular polarity.

Goals
- Determine bond type using electronegativity values
- Indicate bond polarity with a polar arrow or partial charges
- Rank bonds in order of polarity
- Predict molecular polarity using bond polarity and molecular shape
- TL: some physical property sense-making like electric field interactions, mp, bp, or solubility?

Student difficulties
RP: My own experience is that students in first year General Chemistry at the University level are reasonably comfortable with the concept of polar covalent bonds, and appreciate that there can be a continuity between purely ionic and purely covalent bonds. They most frequently run into trouble when they try to pass from the polarity of individual bonds to the polarity (or lack thereof) of a molecule as a whole. That is, they have a reasonable grasp of the isolated concept of "bond polarity" but have difficulty integrating it with more general concepts of chemical structure.
We have some data from the General Chemistry Concept Survey which has been given to our Gen Chem I students since 2007. This survey contains several questions related to bond polarity. I have attached some results below:

General Chemistry I Concept Survey
Excerpt: questions related to bond polarity

11. *In the XeF2 molecule there are 3 non-bonding electron pairs around the Xe atom. Which of the following statements about the polarity of this molecule is correct?*

a. Non-polar because of the difference in electronegativities.
b. Non-polar because of the shape of the molecule.
c. Polar because of the 3 non-bonding pairs.
d. Polar because of the shape of the molecule.
e. Polar because of the difference in electronegativities.

	Pre, Fall 2006	Post, Fall 2006	Pre, Fall 2007	Post, Fall 2007
Student % correct	NA	NA	10.4%	17.7%
Disc. Factor	NA	NA	0.4	19.7
TA % correct	NA	NA	50.0% **(9x)**	66.7% **(6x)**

14. *Select the* ***non-polar*** *compound(s), if any, from the choices below:*

CH3Cl *CCl4*

a. CH3Cl is non-polar
b. CCl4 is non-polar
c. Both are non-polar.
d. Neither are non-polar.

	Pre, Fall 2006	Post, Fall 2006	Pre, Fall 2007	Post, Fall 2007
Student % correct	NA	NA	35.2%	60.8%
Disc. Factor	NA	NA	29.0	42.3
TA % correct	NA	NA	100.0%	94.4% **(1x)**

15. *What is the reason for your answer to question 14?*

a. Both molecules contain polar bonds so they are polar.
b. Both molecules contain carbon, so they are non-polar.
c. CCl4 has polar bonds but the shape cancels the individual bond dipoles.
d. CH3Cl has polar bonds but the shape cancels the individual bond dipoles.
e. both (c) and (d)

	Pre, Fall 2006	Post, Fall 2006	Pre, Fall 2007	Post, Fall 2007
Student %	NA	NA	34.4%	60.8%

correct				
Disc. Factor	*NA*	*NA*	*27.9*	*42.9*
TA % correct	*NA*	*NA*	*100.0%*	*94.4%*

18. *The bond in HF is described as polar covalent because:*

a. electrons are centered on the fluorine and protons are centered on the hydrogen.
b. the bonded electrons can always be located between the two nuclei.
c. there is a negative charge on the fluorine atom because it has more valence electrons.
d. there is a –1 charge on the fluorine because it gained one electron.
e. there is greater electron density on the fluorine because it is more electronegative.

	Pre, Fall 2006	*Post, Fall 2006*	*Pre, Fall 2007*	*Post, Fall 2007*
Student % correct	*31.6%*	*73.4%*	*21.5%*	*69.1%*
Disc. Factor	*23.0%*	*25.4%*	*19.6*	*30.5*
TA % correct	*NA*	*NA*	*100.0%*	*100%*

20. *Consider a molecule with the formula ZA2 where Z is the central atom and A and Z have different electronegativities. In which of the following cases would this molecule* ***always*** *be nonpolar?*

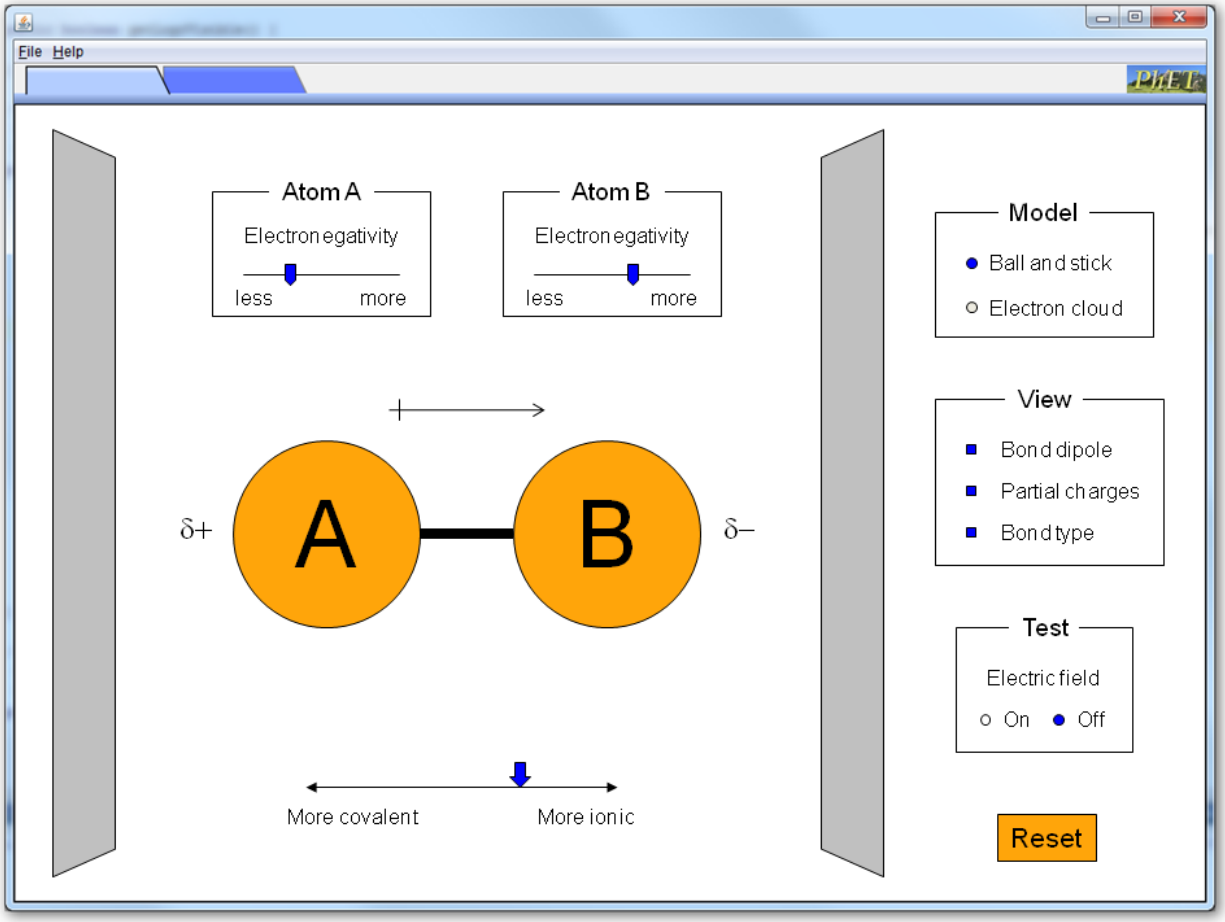
a. If each A has 2 lone pairs and Z has no lone pairs.
b. If Z has 2 lone pairs and each A has no lone pairs.
c. If Z has 1 lone pair and each A has 3 lone pairs.
d. If A is drastically more electronegative than Z.
e. If Z is drastically more electronegative than A.

	Pre, Fall 2006	*Post, Fall 2006*	*Pre, Fall 2007*	*Post, Fall 2007*
Student % correct	*23.6%*	*43.8%*	*24.1%*	*40.0%*
Disc. Factor	*2.2%*	*23.8%*	*14.1*	*31.5*
TA % correct	*NA*	*NA*	*61.1%* **(7x)**	*88.9%* **(2x)**

Mockup

In this sim, students can change polarity and see the effects of polarity.
Note: In first 2 tabs, make the atoms different colors.

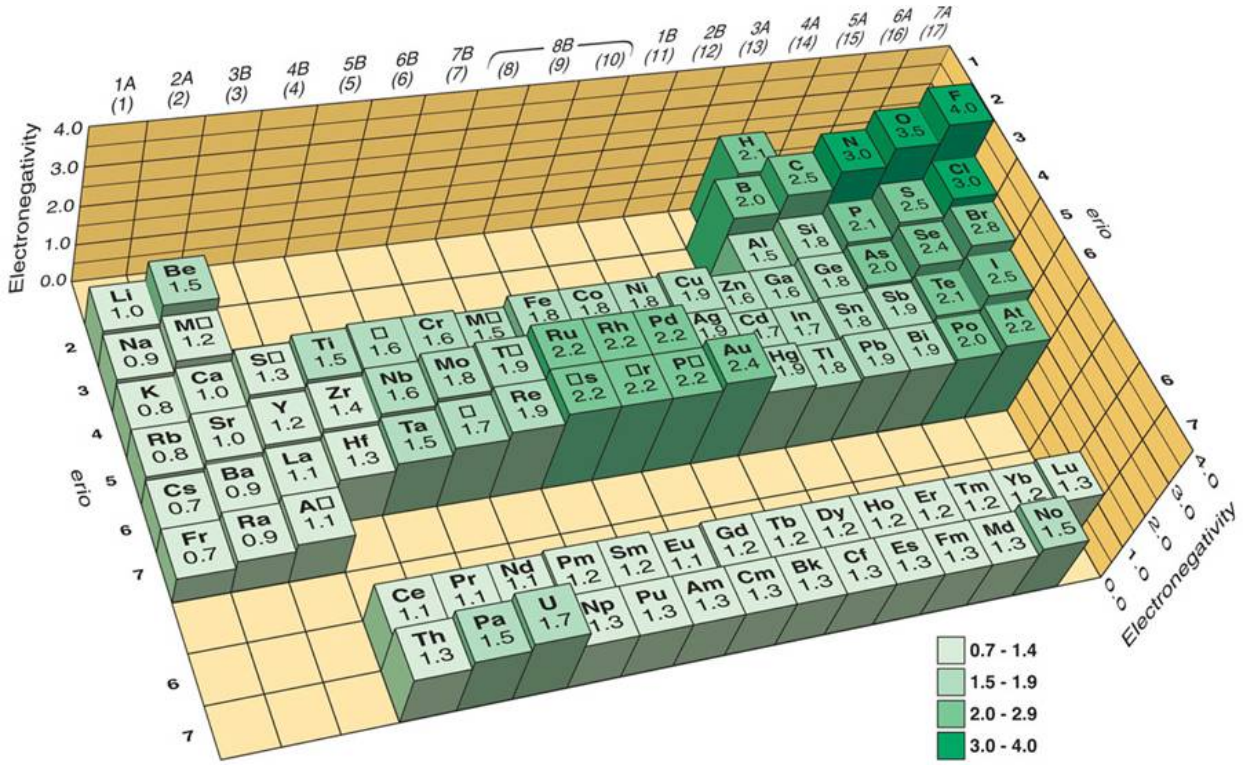
Tab One: 2-atom molecules



Change electronegativity

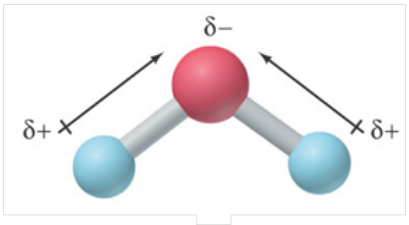
Students can use a slider to change the EN of each atom. EN is the ability of a bonded atom to attract the shared electrons. Below is a chart of relative EN values. The max value is 4.0; the min value is 0.7. Should the slider go to zero? Should we show the EN values?

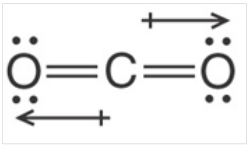
Update: snap to tick marks

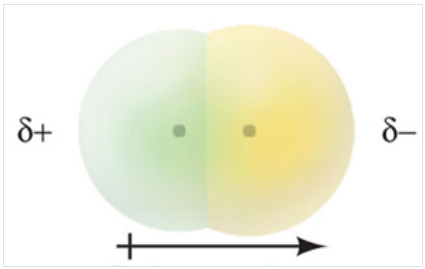


Show bond dipoles

The arrowhead points to the negative pole and the tail is crossed to make a “plus”. Below are some examples. The size of the arrow is proportional to the dipole, and the direction of the arrow is along the bond..







CM: Is the student expected to know the representation for dipoles? I never would have been able to interpret this from the sim.

KL: No, but students can learn this representation by using the sim and comparing the arrow head and tail to the partial charges.

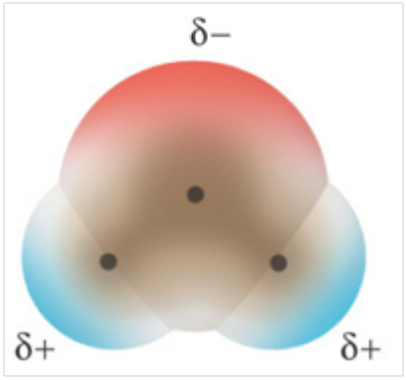
CM: I’ll be really surprised if “using the sim” leads to the conclusion that the cross at the arrow tail means “positive” and the arrow head is therefore negative.

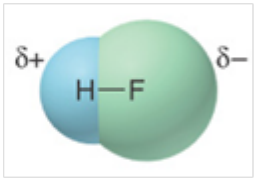
KL: By interacting with the sim, and changing the polarity, I think students will develop a working definition for the bond dipole (and the arrow that represents it).

Show charges

The lowercase letter delta represents partial charge. Below are some examples. Should the size of the letter be inversely proportional to the charge? That is, the closer the partial charge

is to a “full” charge, the smaller the letter delta? No, the size of the letter should be directly proportional to the charge.





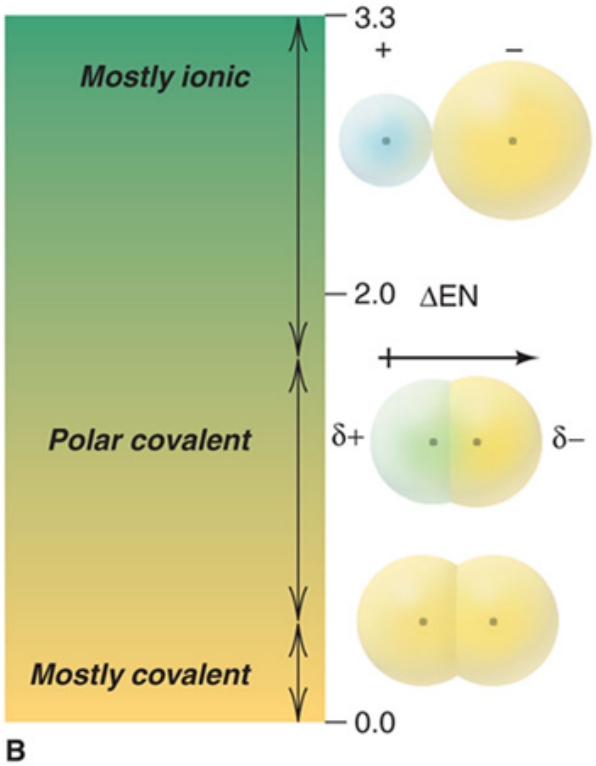
CM: Is the student expected to know these representations for charge?
KL: Is your concern with the delta symbol?
CM: Yes, concern is with the delta. Who is the audience? (I don’t see that in this doc.) Will they be familiar with Greek characters, know that this is delta, and know that delta means difference? For example, we engineers are used to seeing delta as a triangle.
KL: See “audience” under learning goals. I am not sure students will be able to say “this is delta”, but they will learn that is what we chemists use to represent partial charge.
CM: But how will they learn it solely from the sim? Seems like prompting or scaffolding is needed. Same with the dipole representation.

See: The Origin of the “Delta” Symbol for Fractional Charges
W.B. Jensen, J. Chem. Educ., 2009, 86 (5), p 545

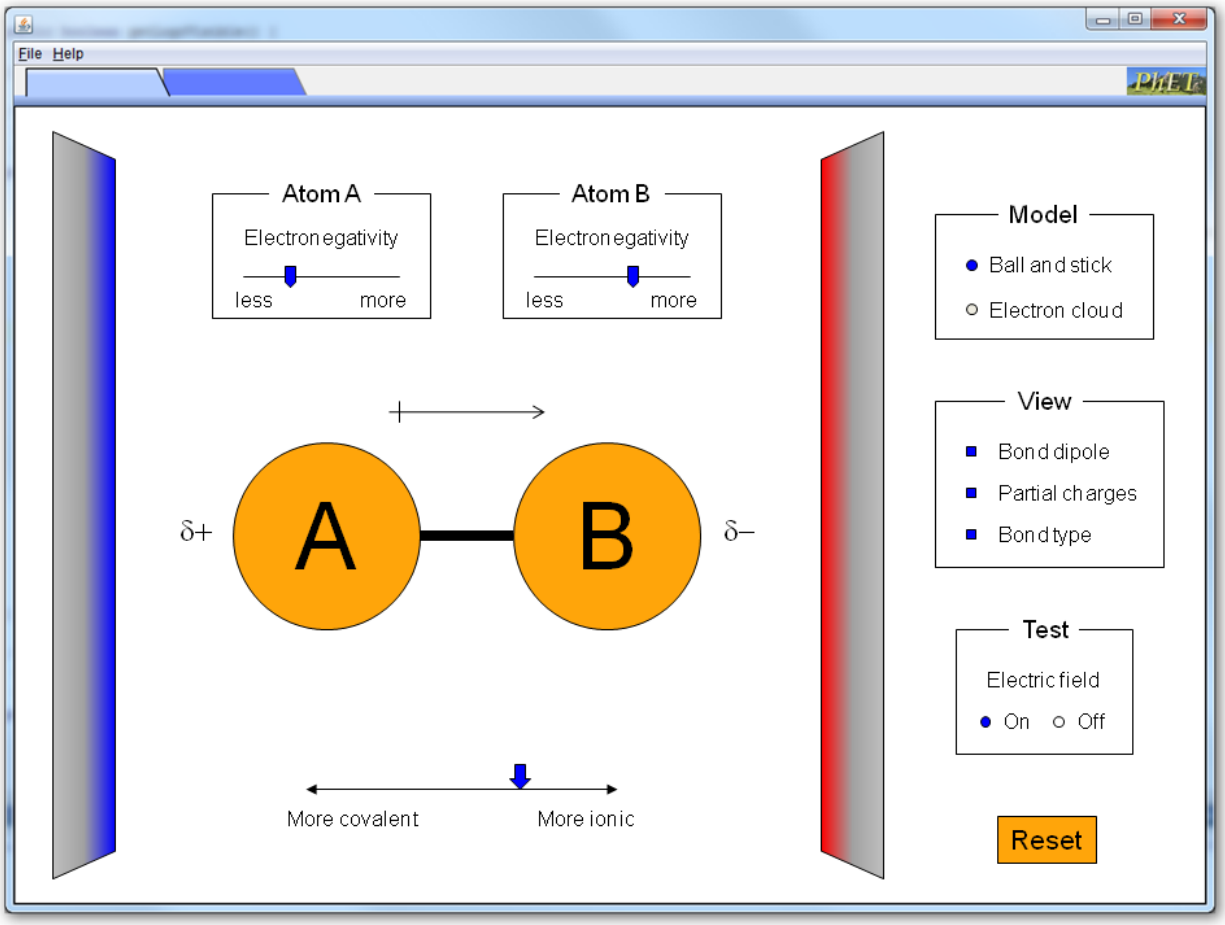
Show bond type
A dial shows if the compound is “more ionic” or “more covalent.”

ΔEN	IONIC CHARACTER
>1.7	Mostly ionic
0.4-1.7	Polar covalent
< 0.4	Mostly covalent
0	Nonpolar covalent

A

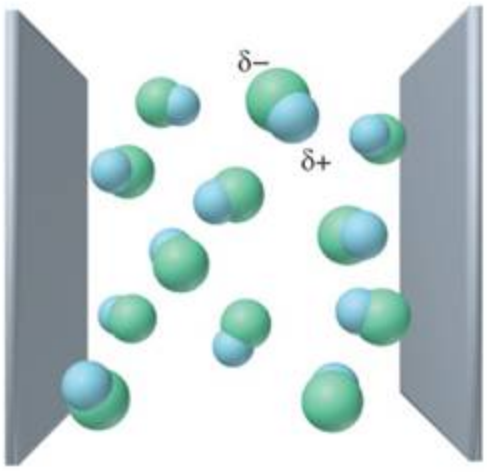


B

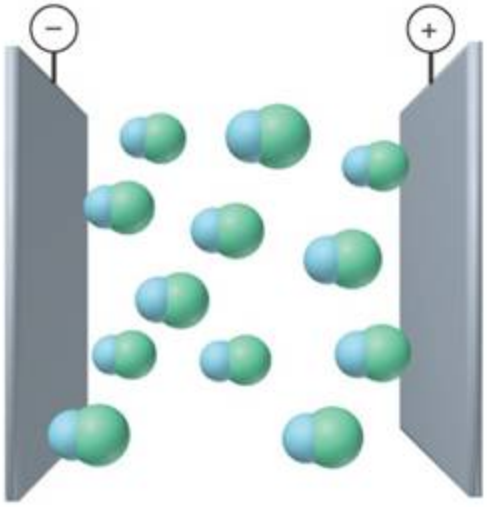


Electric field off/on

The orientation of molecules in an electric field depends on polarity. Below is an example.

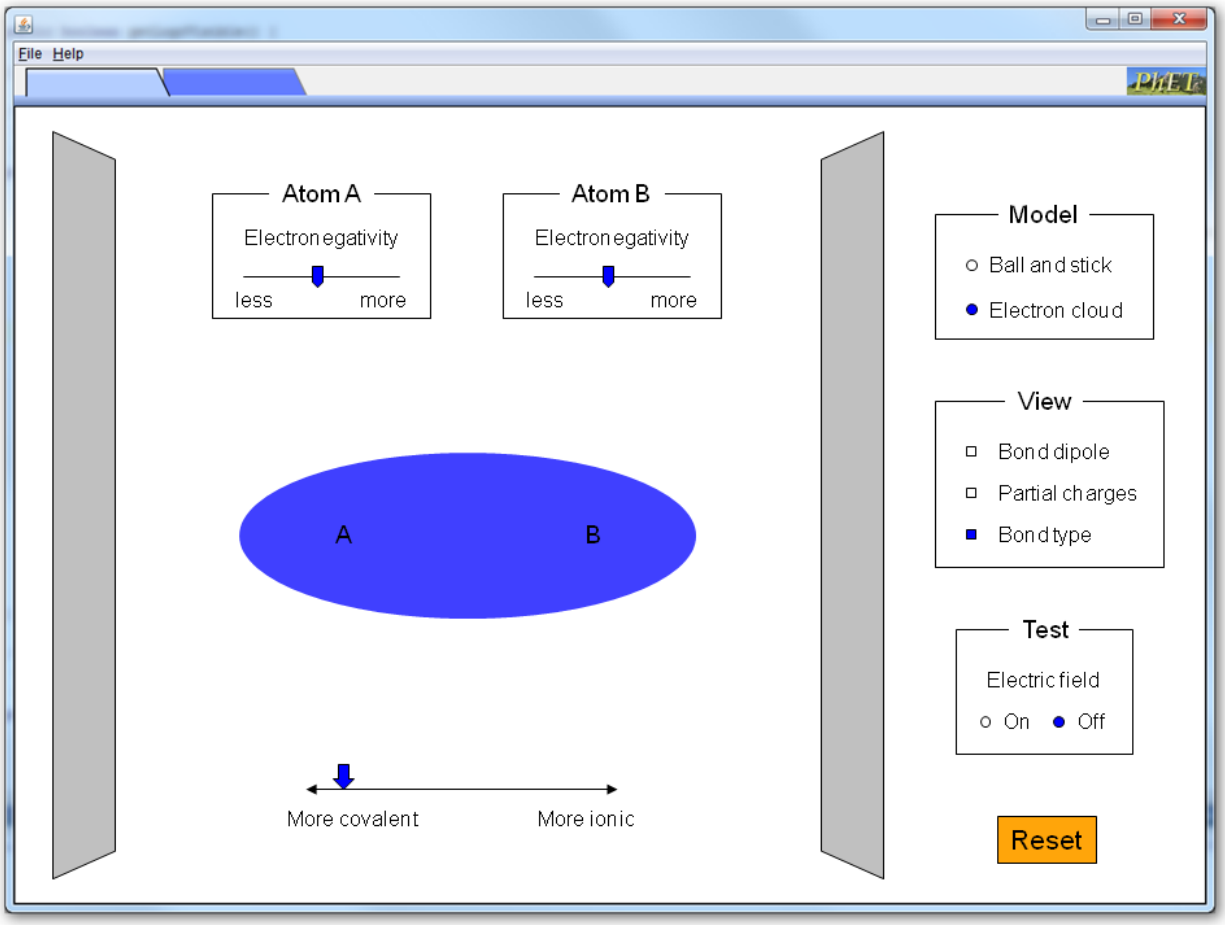


B Electric field off



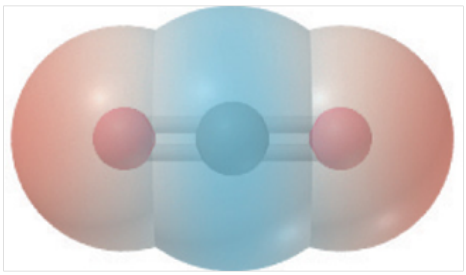
C Electric field on

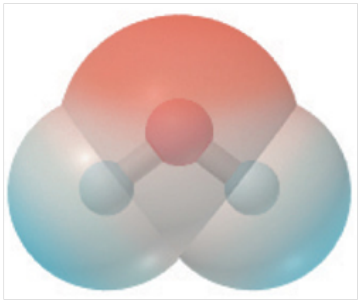
CM: Should the plates be labeled positive (+) and negative (-)? Why is only part of each plate colored? Is charge only on the back third of the plate?
KL: Yes, the plates should be labeled, and no, the charge is on the entire plate. The color is an attempt to give students another visual indicator that the electric field is on. Do you have other ideas?
CM: Color the entire plates when the E-field test is on, and mark them with + and - as in the section “Electric field off/on” above.



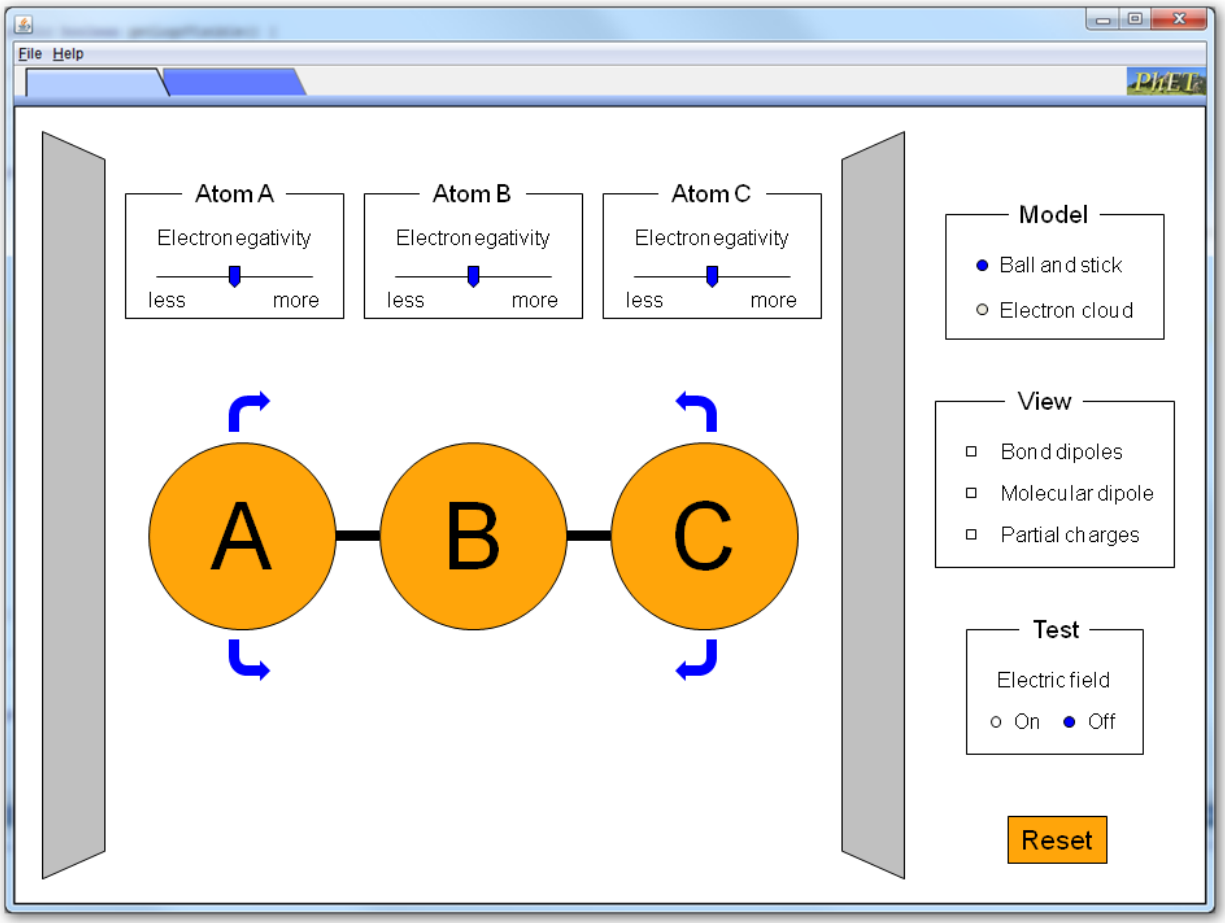
Show electron density

This shows regions of high electron density (red) and low electron density (blue). Below are some examples. Another option is to show the electron cloud shift with EN. We need to discuss!





Tab Two: 3-atom molecules



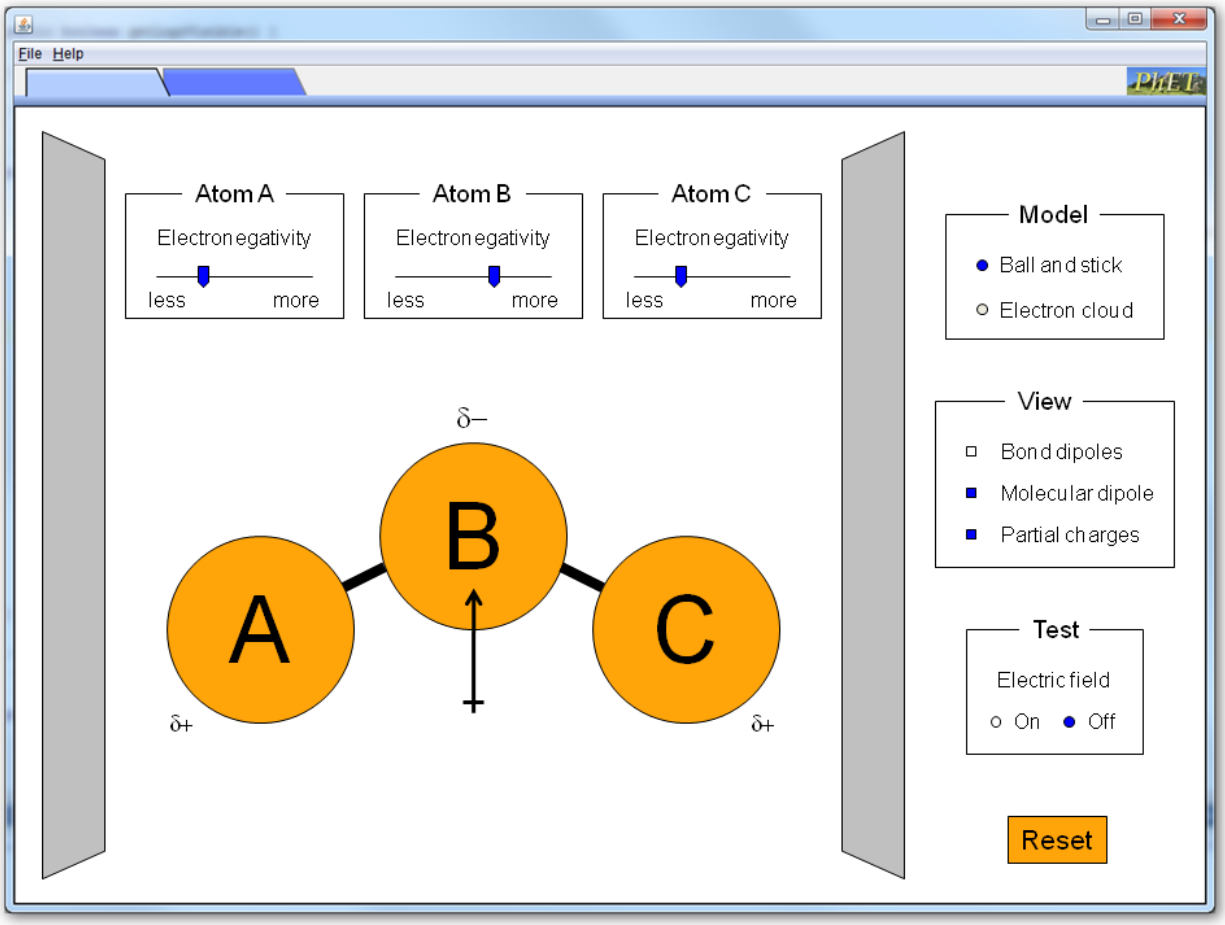
Change shape (or angle)

Two ideas: 1) students can interact with the atoms directly, or 2) students can use a slider that changes the angle. Try option one first. The bond *length* should not change.

CM: What do the blue arrows mean?

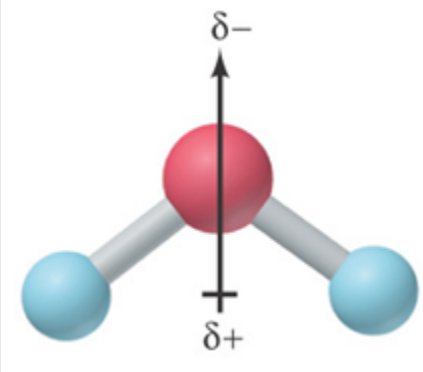
KL: The arrows are not visible to students, they are meant to indicate that students can drag the outer atoms up or down.

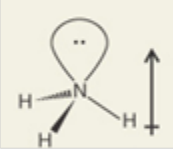
CM: OK, I see... they are drag handles to change the angle. I think we should change the cursor to this type of arrow on mouseover.



Show molecular dipoles

This is the same polar arrow used for bond dipoles, but now there is only one per molecule (the molecular dipole is the sum of the bond dipoles). Below are some examples.





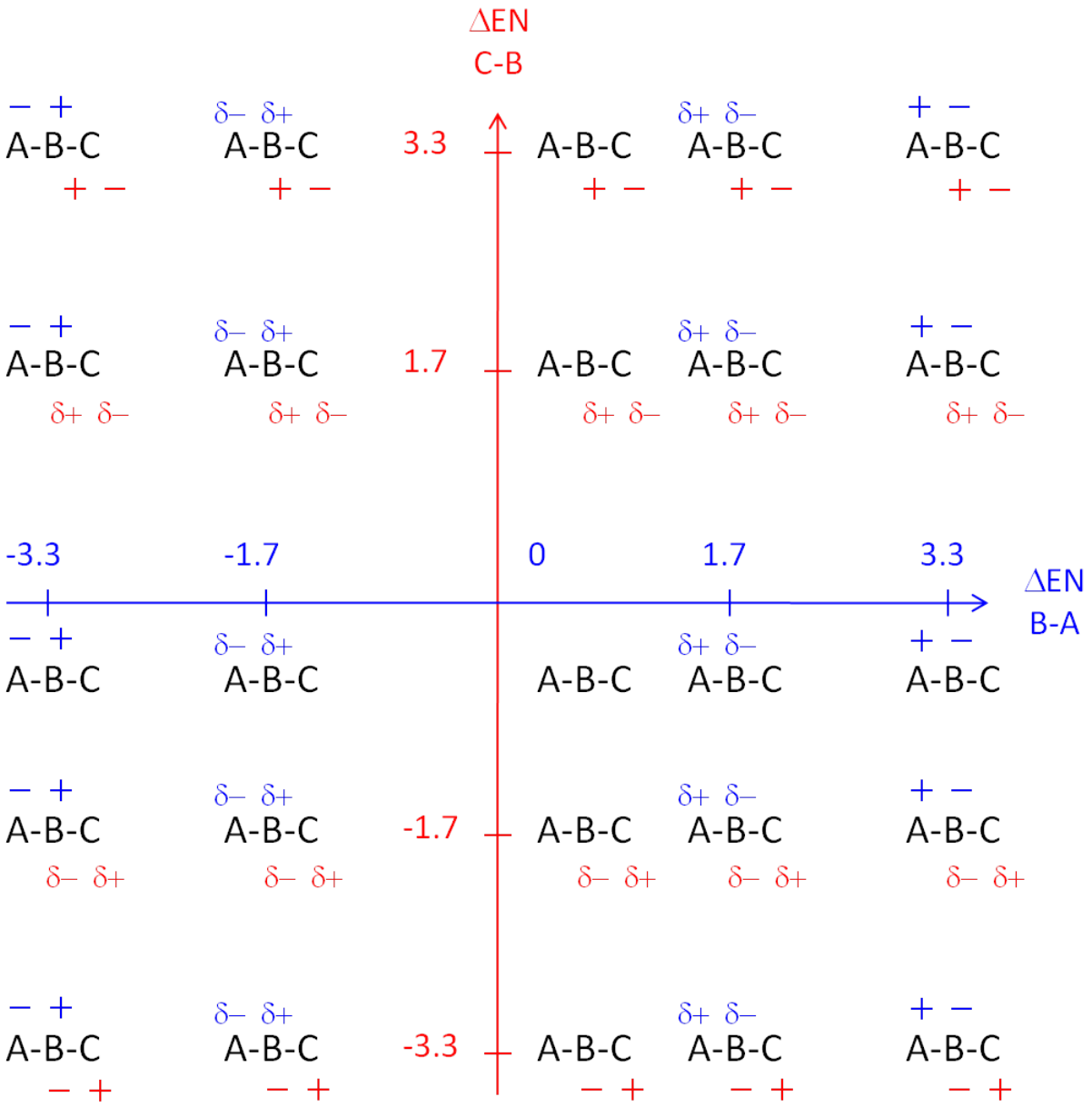
CM: Bond dipoles and molecular dipoles use the same representation. Do these View options need to be mutually exclusive? (radio buttons instead of check boxes)

KL: Yes, they use the same representation, but students should have the option to see both at the same time.

CM: OK. Maybe they should be different colors, and we can put the arrows next to the check

boxes?
KL: Yes, good idea on the arrow icons.

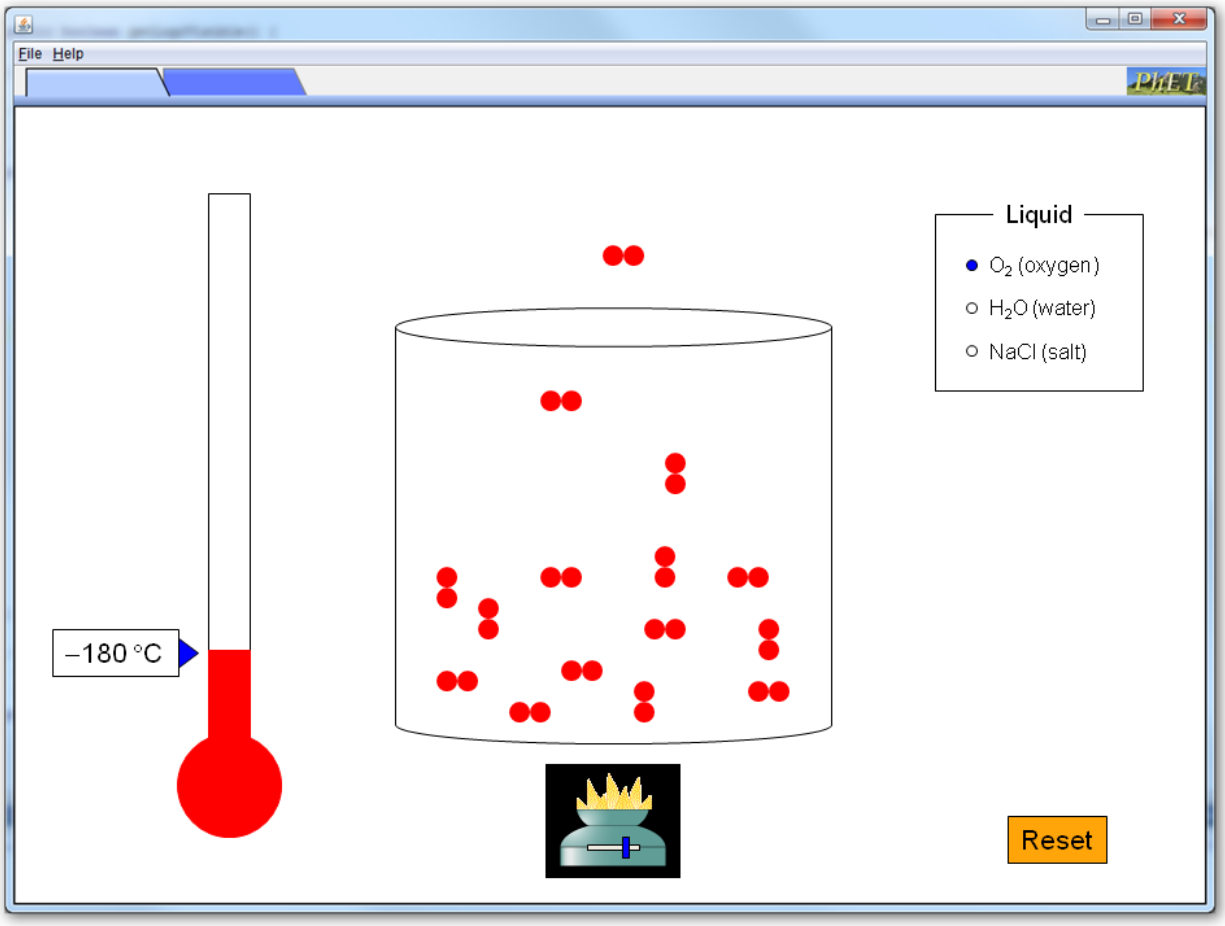
Model
- need to convert EN difference to partial charge; fine for 2-atom case, but 3-atom case is complicated
- could treat A-B and B-C independently (see below), but need to consider 3-atom interaction to account for the polarity of O3
- can get ionic and covalent bonds in same molecule; could limit the range of EN values



Tab Three: Real molecules

Need to mockup!

Tab Four? Boiling Point



Measure boiling point

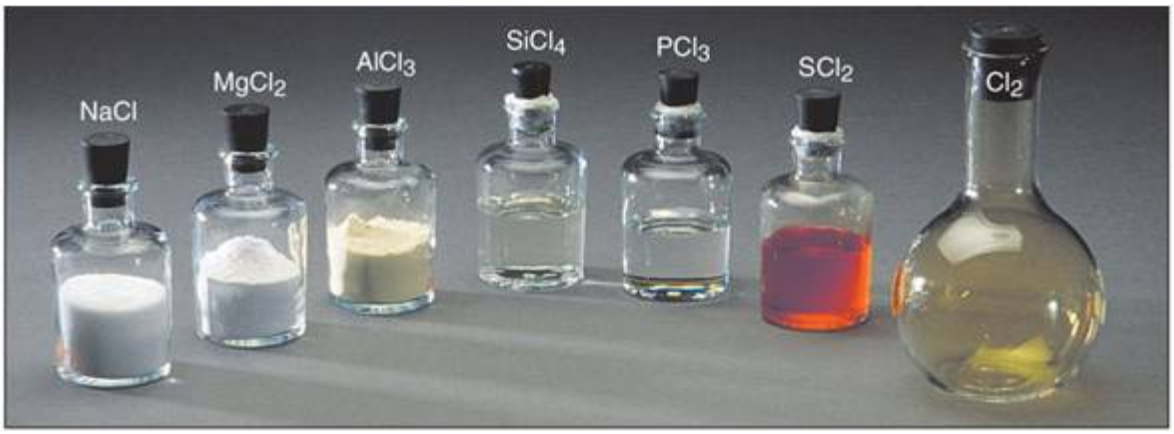
Students can add heat and see a liquid become gas. See the States of Matter sim for an example. They can measure the BP with a thermometer (default units = C). Below is a table of melting and boiling points.

Compound	Type	MP (C) @ 1 atm	BP (C) @ 1 atm
LiF	ionic	845	1676
NaCl	ionic	801	1412

KBr	ionic	734	1435
HF	polar	-84	20
H2O	polar	0	100
NH3	polar	-78	-33
H2	nonpolar	-259	-253
O2	nonpolar	-219	-183
CH4	nonpolar	-182	-162

Test solubility

Students can test the solubility of the compound in water (at STP). The phase of the compound at STP depends on its polarity. Below is an example of third row chlorides.



History

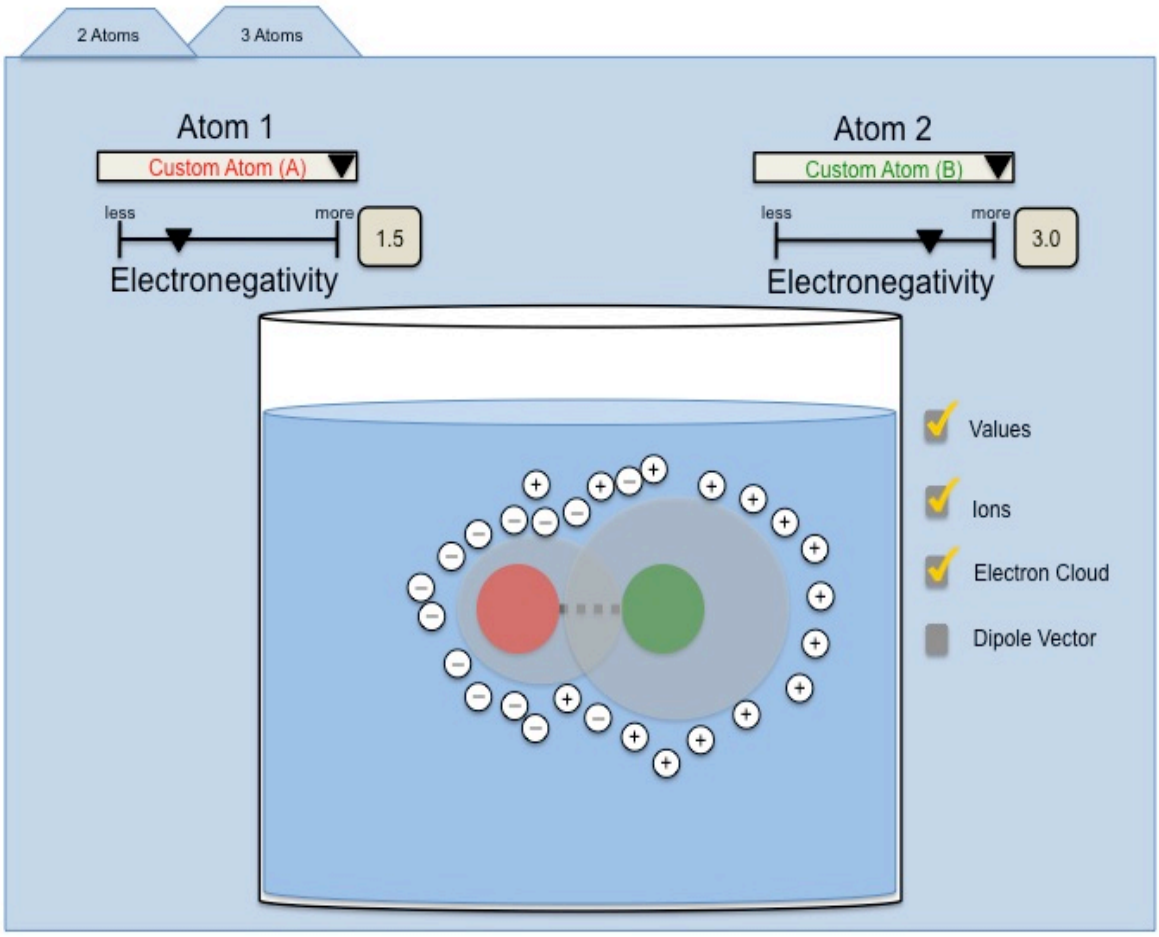
See Jack B mockup below.

Polarity

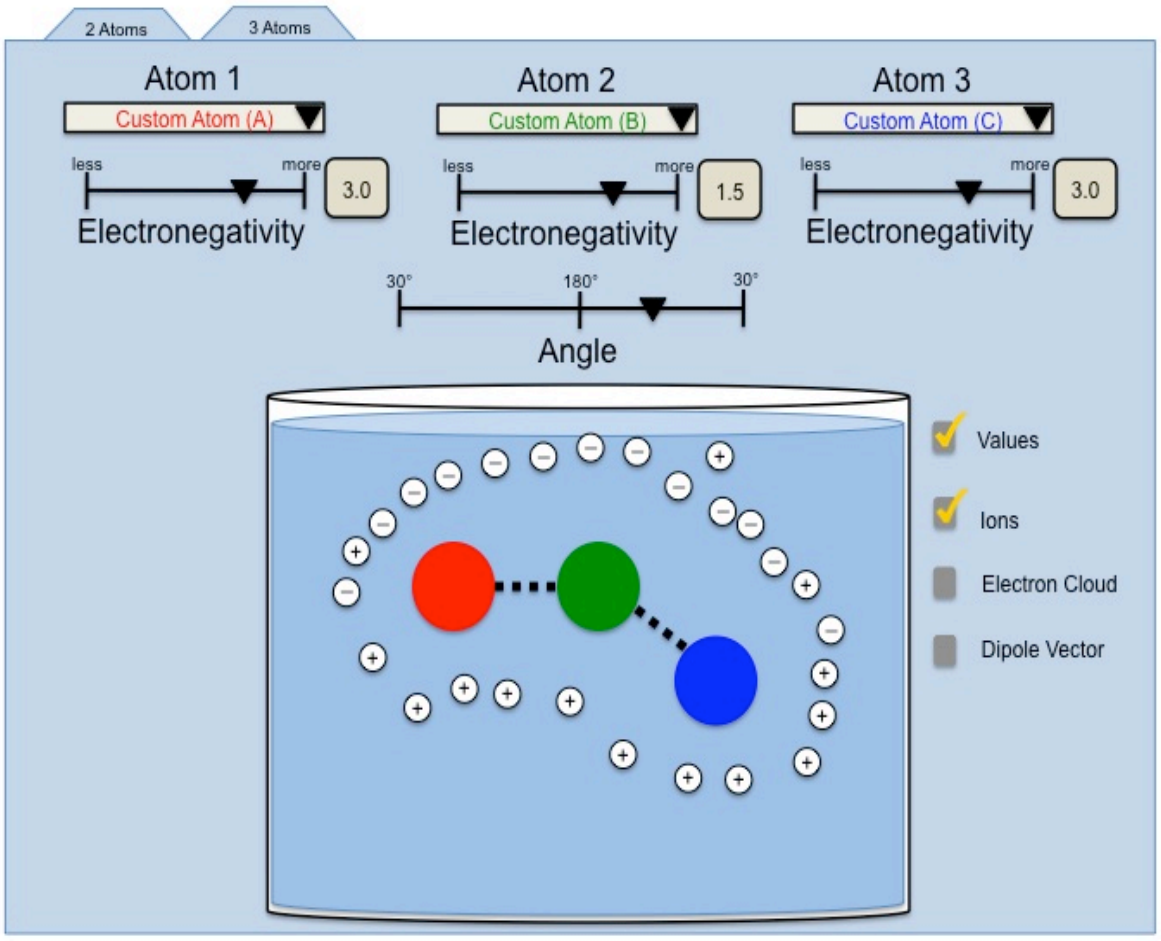
- Allows user to discover how electron density effects bond and/or molecular polarity
- Tab 1 (Two Atoms), bond polarity only
    - Controls
        - each atom has its own slider which varies electronegativity
    - Each atom in the model will have a "cloud" of electrons which moves as electronegativity changes
    - Display can indicate if electrons form an ionic or covalent bond
- Tab 2 (Three Atoms), bond and molecular polarity of covalent species
    - Controls

            - each atom has its own slider which controls electronegativity
            - separate slider controls angle between the three atoms
                - default = 180°, range = +/- 30°
- Ideas for how to indicate uneven electron distribution (polarity)
    - Electrolyte Solution (shown in mock-up)
        - cations (+) and anions (-) will surround electron clouds based on electron distribution
        - as electronegativity or angle is adjusted, ions will rearrange to new positions based on new polarity
        - when di- or tri-atom in non-polar, ions will be randomly distributed
    - Add a detector, like in the "charges and fields" sim, to indicate charge at a point
        - User can move detector around and see how charge varies based on where they are in the cloud
    - Readout to measure "effective charge" on each atom
        - Example:
            - non-polar diatomic, effective charge on each atom = ZERO
            - polar (covalent) diatomic, atom charge displayed as a fraction, sign indicates + or -
            - ionic, atom charge displays as + or - ONE to indicate gain or loss of an electron
    - Bond polarity vector arrows
        - default = OFF
        - user can click on to show vector arrow
    - Molecular polarity vector arrows
        - default = OFF
        - user can click on to show vector arrow

Polarity: Tab One



Polarity: Tab Two



Online Resources

Wikipedia article on chemical polarity.

Other Sims

TL: This has a nice way to show electron density. Also there are many interesting sims on http://mw.concord.org/modeler/. Run the chemical bonding sim.

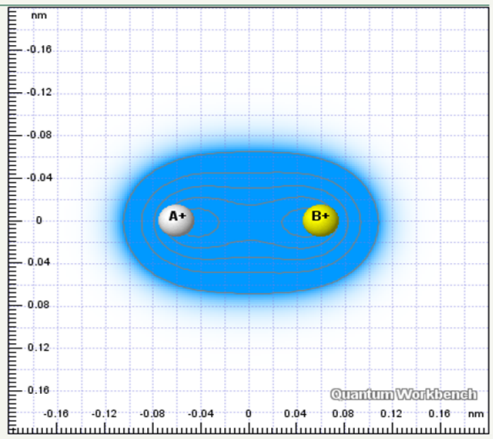
The polarity of a diatomic molecule

The model to the right shows a diatomic molecule initially consisting of two identical atoms. Two sliders are provided below for changing the atoms to ones that have different electronegativities.

Instructions:

1. Click the "Run" button and observe the movement of the electron clouds.
2. Adjust the sliders so that the atoms' electronegativities are different and observe what happens. Repeat this for a number of different settings.

Note: **Be sure to let the model run for a few seconds and do not move the nuclei in this model.**



Electronegativity of atom A

1 2 3 4

Electronegativity of atom B

1 2 3 4

Run | Stop | Reset cloud | Take a snapshot | ☑ Contour | ☑ Grid

The polarity of a triatomic molecule

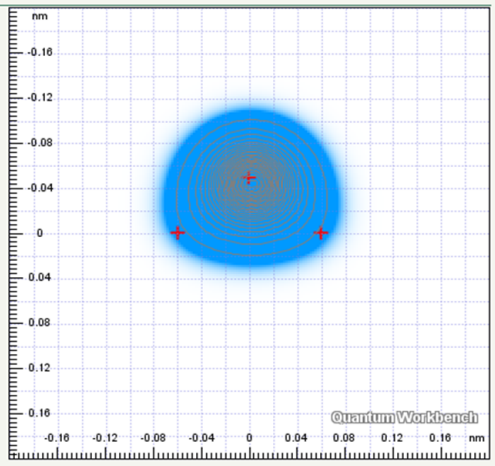
Polarity can also arise from the asymmetric arrangement of atoms in a molecule. In the model to the right, there is a triatomic molecule with three nuclei initially placed in a line.

Instructions:

1. Click the "Run" button and observe the movement of the electron cloud for a while.

2. Use the "Vertical position of the middle atom" slider to adjust the position of the central atom until the triatomic molecule has a conformation that looks like a H_2O molecule:

Be sure to let the model run for a few seconds between each move.

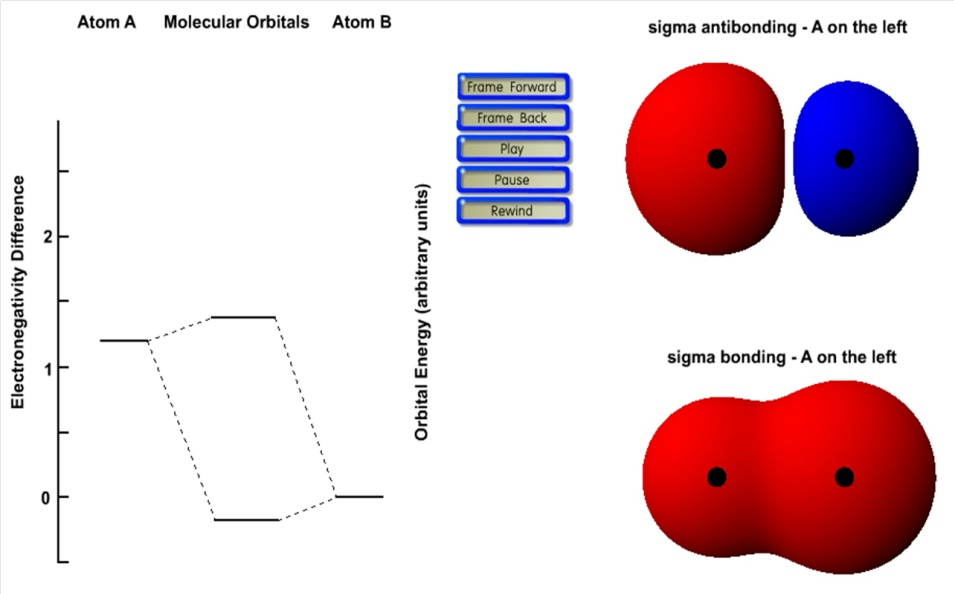


The vertical position of the middle atom (nm)

Run | Stop | Reset cloud | Take a snapshot | ☑ Contour | ☑ Grid

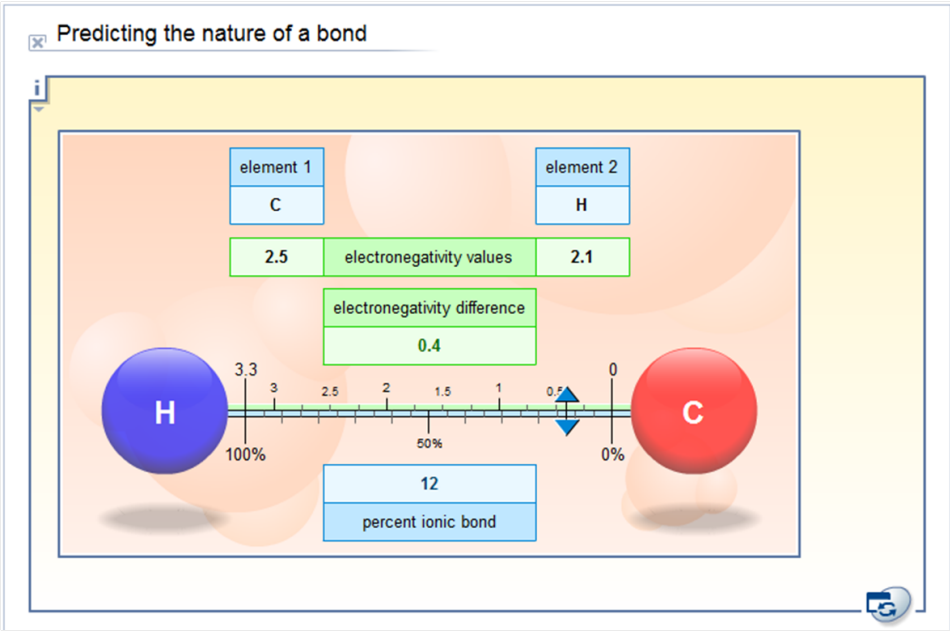
-0.1 0 0.1

KL: This animation was shown in a talk at the GRC:
http://www.wellesley.edu/Chemistry/Flick/chem341/mocovtoionic2.html



http://www.chem.iastate.edu/group/Greenbowe/sections/projectfolder/flashfiles/reaction/bonding1.html

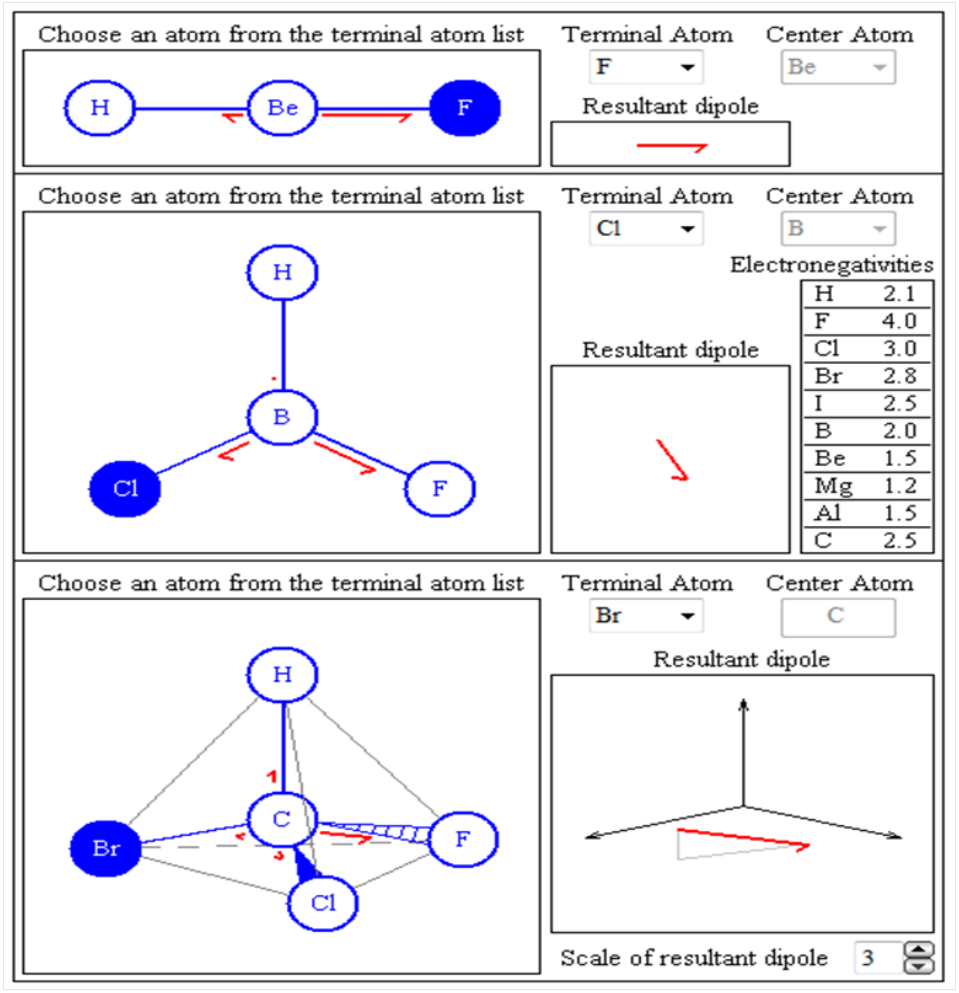
http://www.yteach.co.uk/index.php/resources/electronegativity_polarity_variation_periodic_table_group_bond_t.html



JC: I tried the above sim; it seems like a useful tool (you have to enter numbers, no dragging sliders) but after one use I got a big “You must buy a licence” message. If/when you try it out,

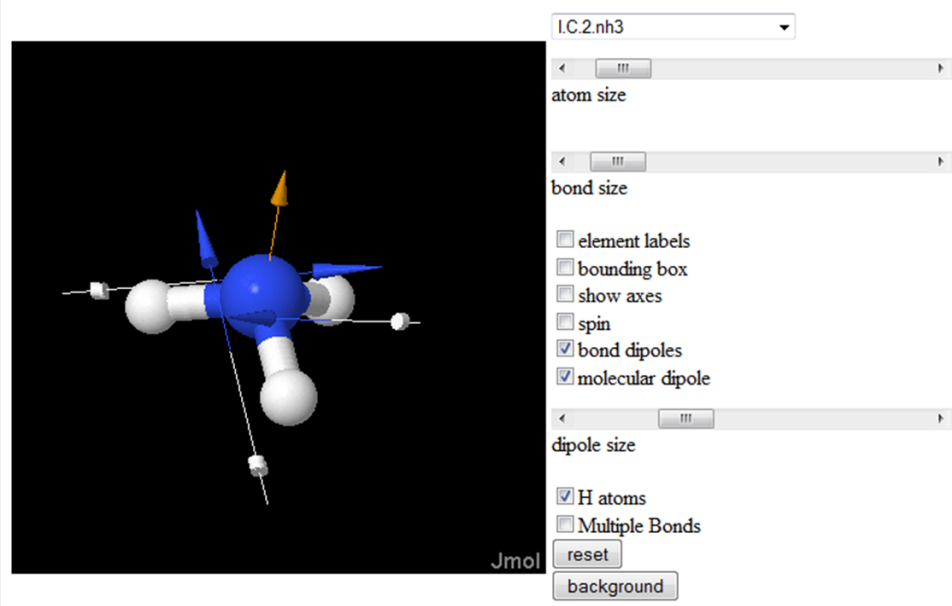
observe as much as you can on your first use.

http://www.media.pearson.com.au/schools/cw/au_sch_derry_ibcsl_1/int/molecularPolarity/1003.html



EM: I met someone at a conference this weekend who has used Jmol to show dipoles in some simulations.
Here's a link to the sim http://genchem1.chem.okstate.edu/ccli/StartUp.html (you have to put in a name and email address, and then you can access the sims. No special login needed. For Mac users, the sims only work with Safari.)

Once you have entered your name and email, go to "Personal MoLE Page Access", "Web-based simulations". Then search for 'Jmol' to find the sim.

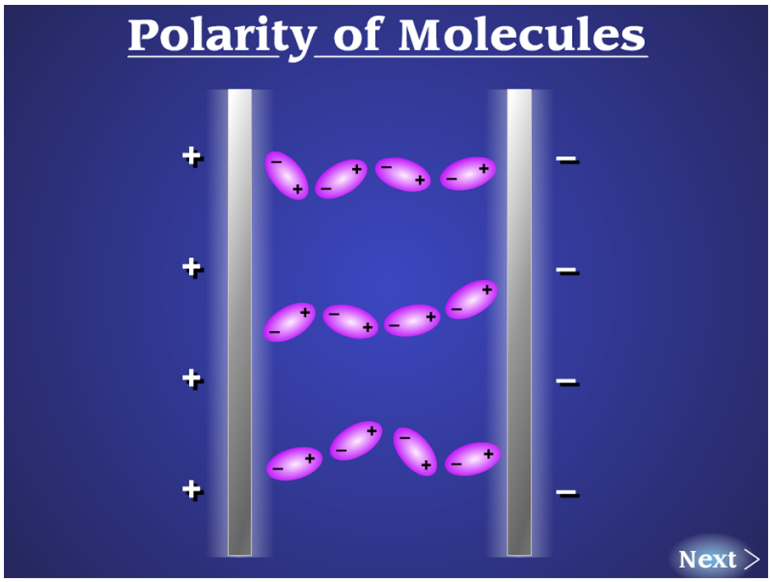


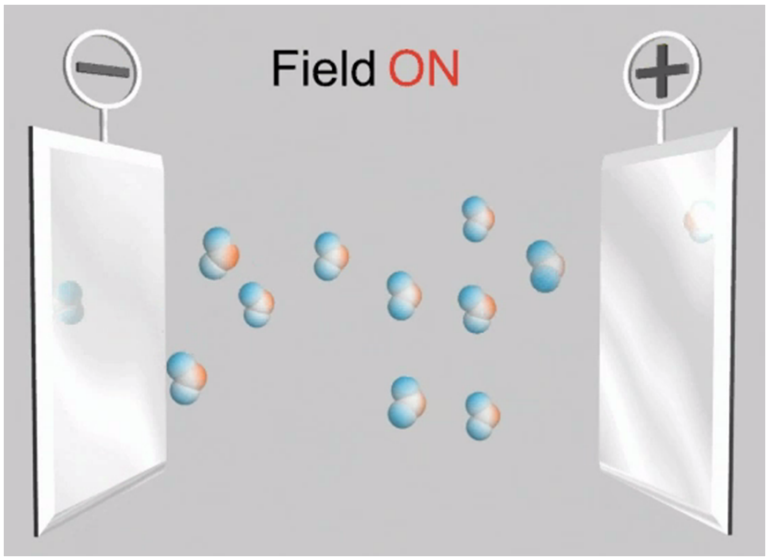
EM: Here's another sim that allows building in 3D (though doesn't show dipoles)
http://www.sciencegeek.net/eChem/eChem.html
I like that you can rotate the molecule and add atoms. The interface is unbelievably clunky. I had to download the manual to figure out how to actually build anything.
-To make methane, click on 'construct' then a pink-ish window should appear. At the bottom, where it says "select molecule to edit" choose 'build new molecule'. A window should pop up that allows you to name the molecule (apparently whatever you want). Then select "atoms" from the left-hand side, select Carbon from the right-hand side, then select the appropriate geometry (tetrahedral). Then select inside the play area, and a ball with four sticks coming out should appear. Select H from the right-hand side, then one of the sticks coming off the Carbon in the play area, and this allows you to add hydrogen. Keep doing that until you get methane.

CM: Wow, that really is a horrible user interface. It looks like there are some bugs in the molecule rotation algorithm, too. Shouldn't be too hard to do better than this.

CM: Here's a page that "illustrates the new capabilities of Jmol to calculate and display dipoles and simple arrows."
http://chemapps.stolaf.edu/jmol/docs/examples-11/dipole.htm

KL: These animations are from the Silberberg textbook.
http://www.mhhe.com/physsci/chemistry/animations/chang_7e_esp/bom4s2_7.swf





Literature

Difficulties with the Geometry and Polarity of Molecules: Beyond Misconceptions
C. Furió and M. L. Calatayud, J. Chem. Educ., 1996, 73 (1), p 36
- poor English
- need to predict molecular shape correctly before you can predict polarity
- some students only use the shape, some only use the polarity of the bonds
- what about ozone? only has O atoms, but polar

Using Computer-Based Visualization Strategies to Improve Students' Understanding of Molecular Polarity and Miscibility
Michael J. Sanger and Steven M. Badger II, J. Chem. Educ., 2001, 78 (10), p 1412
- do electron density plots help? yes, if topic involves electronic charges on molecules

- did a control study - students *viewed* “elpot” maps

Teaching Ideas

Activity
Write here.

Assessment
See Chemical Bonding in Picturing to Learn.

Interview Feedback

KL will add interview notes here. KL will use some of the questions from the concept survey in the interviews.

Discussion

04/07/11 - First team meeting

- KP: in custom mode, see electron cloud (blue) shift as you change electronegativity - KL: how to represent cloud? KP: cloud gets darker & bigger - KL: dots for the nuclei
- RP: could also select elements from PT - KL: but may not make a molecule - KP: could choose a diatomic, see where it is on PT
- KP: checkbox for “show net charge” - KL: needs to be outside of cloud
- KP: should we show if ionic or covalent? KL: no clear distinction - RP: could use a dial for “more ionic” or “more covalent”
- KP: checkbox for electronegativity values - off by default
- KP: what representation to use for molecule? KL: need ball & stick and electron cloud
- KP: tabs could be: 2-atom, 3-atom, and real molecules - in 3-atom tab, could use another dial for “polar” or “nonpolar”
- KL: how to represent boiling? TL: maybe use magnifying glass to address micro-macro issue - KP: Kelly and Emily will discuss
- KL: should we allow students to test solubility in water? KP: could use an indicator that says “soluble” or “not soluble” in water
- KP: would be nice to have sim where you can mix 2 diatomics with ability to change polarity - also real mixture like oil and water - RP: oil is large, could use pentane - EM: over time, could see them separate

06/02/11 - Second team meeting

How to map EN difference to partial charges (or dipole)?
- EM: figure out max, go from there
- KL: what about 3-atom case? if all atoms are the same, the central atom will have a partial charge (ozone example)
- KL: we also ignore lone pairs on the central atom

How to represent partial charges?
- size of delta changes; no delta when ionic
- CM: can we say “partial charge” when ionic? KL: maybe only ionic when EN at extremes
- use red for + and blue for -

Can students rotate the molecule?
- in 2-atom case, rotate around center of bond
- in 3-atom case, rotate around B (central atom) KL: if mouse-over B, see curved arrow EM: do we need to rotate in 3-atom case?
- KL: then we can use the speed of motion (when E-field is on) to indicate polarity CM: like compass in Faraday sim

Do we need a “real molecules” tab?
- KP: could show location on PT to give context
- KL: in that case, can we use 3D? CM will ask JO about Jmol
- KP: how about a “mystery molecules” tab for teachers?

How to show intermolecular (macro) effect of polarity?
- KL: measure boiling point? EM: hard to represent phase changes
- KL: show physical state at STP? RP: could show macro picture EM: would need outside help to connect with polarity
- KP: list MP, BP in real tab?
- KP: or a bin of diatomics, can change polarity and see how they orient EM: they would not orient, but could see liquid phase expand/contract
- KL: test solubility in water?

Should the cloud change shape?
- KL: it’s nice to see the cloud shift as you change EN, but it’s wrong
- could use electron density (with red and blue shading)
- CM: can students interact with the cloud? KL: can move nuclei
- KL: also nice to have model of bonding other than ball-and-stick

06/02/11 - 3D followup

CM: Following up on our conversation today about potential use of 3D and Jmol in the Polarity sim...
I talked with Jonathan, and here's what I found out:

Jmol was designed for embedding molecules in HTML. It's configured and driven using an awkward scripting language. PhET's use in "Build A Molecule" (BAM) is unusual. It's working well for the limited use in BAM, but skeptical that it's a good general solution.

Jmol might provide a means of inserting addition things (vectors, labels,..) into its scene, but not sure. This would need to be investigated, and a Google search found a few starting points. Let me know if you want me to investigate this.

Using Jmol directly in the play area might be possible, but would need to be investigated. Lots of issues: Jmol has a right-click menu that would need to be disabled (not currently disabled in BAM), we'd need to figure out how to make the background transparent, Jmol is slow to start up, etc. I'm guessing that this integration will be problematic and quirky. Let me know if you want me to investigate this.

Jmol size has been reduced using Proguard, but is still quite large. BAM is 3.2M compressed, but a big chunk of that is the data files that describe geometry of molecules. Don't know exactly how much Jmol is adding to the jar, but it's substantial. Without Jmol, I would expect Polarity's compressed jar to be in the 500K ballpark.

Regarding VSEPR... JO said he really hasn't thought much about it beyond the initial discussion with Emily. At first he was thinking of a 2D organic representation that looks like 3D, but really isn't 3D and can't be rotated. If true 3D is needed, he was going to evaluate how to proceed based on sim requirements.

KL: I do think it is worth investigating the use of 3D and Jmol in the Polarity sim. This issue is going to keep coming up in the chemistry sims because of the 3D nature of many of the concepts.

We may not need to use Jmol directly in the play area. We could show a pseudo-3D representation of the molecule in the play area, and let students click on a button to see 3D in a new window.

BAM has to handle thousands of molecules because students can *build* the molecules. In this sim, students would only be able to *select* the molecules, so the size of the data files should be smaller.

CM: OK, I'll put Jmol investigation on my "to do" list. But I think it makes sense to wait on this until the design (particularly the 3D bits) is a little more fleshed out. Ideally, the design should dictate the tools we use, not visa versa. In reality, it's a tradeoff, but let's not let Jmol's limitations dictate what we do in Polarity.

06/23/11 - 3-atom model

<u>Notes from chem meeting</u>

- no partial charges in 3-atom case OR
- show for each bond, not entire molecule

RP: I came across the following document which gives a prescription for calculating partial charges from electronegativities, but which does takes into account what bonds each atom makes when it becomes a part of the molecule:

http://classes.uleth.ca/200503/chem1000c/charge.pdf - skim or skip the first three pages and concentrate on pages 4-6.

See especially equation 2 on page 4 - perhaps we could use this as our model (internal to the simulation) for calculating partial charges? We wouldn't want to show any numerical values, but this might help us decide whether the central atom for a hypothetical molecule that the students make up by playing with the electronegativities of the atoms, should be delta+ or delta-.

RP: I've been playing with the equation above, and it seems to give qualitatively sensible results. You need to average over resonance structures when counting the lone pair and bond pair electrons for each atom. It's interesting to look at the case where all of the atoms in the molecule are identical (as in ozone.) Then the electronegativities cancel out of the last term, but you still get partial charges which makes sense: the charges are then determined solely by the arrangement of lone pairs and bonds in the molecule. For ozone I get a charge of -1/2 on each outer atom and +1 on the central atom (after averaging together the two resonance structures) which gives no dipole in linear geometry but a dipole moment in nonlinear geometry.

KL: In order to use the equation, you need to know the identity of the atom (for the number of valence electrons), the number of lone pair electrons, and the number of bonded electrons. In our model, the identity of the atom is unspecified, there are no lone pairs, and there is always one bond between atoms (so no resonance structures). I agree that the equation works for real molecules.

07/08/11 - Third team meeting

Issues to discuss:
- title of the sim
- how to show electron density
- model for 3-atom molecule
- interface for 3D in Real Molecules tab
- how to show intermolecular effects (additional tab: Boiling Point, State at RTP, Solubility, JC: Chromatography,... all macro views)

Title
- RP: any PhET guidelines for this?
- Consensus: "Molecule Polarity"

Cloud
- How to represent shift? Size or color?
- CM: hard to implement in 3D
- Consensus: Cloud shift (and naked nucleus) is wrong! KL: but Kathy likes
- KL: color is nice to show how it aligns with red/blue plates
- RP: not able to use cloud shift in 3-atom or 3D
- Consensus (KL, EM, JC, RP, CM): electrostatic potential is better representation
- KP enters: cloud shift seems more visceral, students may not be able to interpret color mapping like experts. EM: but used at intro level. KP: worth doing student interviews
- KP: or no size change, but more/less transparent to show density of electrons & attraction (KL: not blue)
- Need two “cloud” view options

Decided to try 2 “cloud” representations: electrostatic potential view, and electron density view. For the the latter, we may want to use a color other than blue or red, to avoid confusion with the former.

JC: electron density map examples for carboxylic acids (scroll down the page to see):
http://www.chem.ucalgary.ca/courses/351/Carey5th/Ch19/ch19-1.html
I think these were made using the proprietary software “Spartan”, or something similar.
Also, I don’t know if this free software would help, but it seems to have the capacity to do electron density maps in color: http://www.scl.ameslab.gov/MacMolPlt/

3-atom model
- KL: if add partial + charge to central atom, need partial - charge (1/2 size) on outer atoms
- RP (later): equivalent to one tick mark
- Need to show 2 partial charges on central atom
- CM: should you be able to set EN value exactly?
- EM: if quantitative, may compare to PT
- JC: options to lock A & C sliders to same value? and A, B & C?
- RP: need to indicate to students, CM: could use photoshop icon
- KP: Here is the database of triatomic molecules:
http://physics.nist.gov/PhysRefData/MolSpec/Triatomic/Html/appendix.html
- CM: or show/hide EM values?
- No, but snap to value, maybe 10 tick marks (like ruler)

Discussed how to set electroneg of 2 atoms to be identical. Sliders in the design don’t facilitate setting to identical values. Julia suggested a control to make sync multiple sliders together, move one and all move together. Chris suggested a padlock (ala Photoshop) to lock all sliders together. This is getting complicated, so we should probably revisit the sliders themselves. Maybe they should snap to discrete intervals, to facilitate setting identical values? Decided to try ruler-style tick marks (major and minor ticks, unlabeled).

Need to specify internal quantities for electronegativity range (0.7-4), dipole vector magnitudes,

partial charge range, etc.

Real 3D
- JC: maybe show more than one molecule?
- CM: where to put PT? Not in popup. JC: be able to show/hide
- KP: put EN values in PT?
- KL: not sure PT gets “opposite side” idea across

Real Molecules tab will look similar to the 2-Atom tab, with these changes:
• no controls for electronegativity
• combo box for choosing real molecules
• 3D view of molecule, which can be rotated in 3D space
• periodic table somewhere in the play area, atoms in molecule are highlighted, maybe shows electronegativity values of atoms

CM TODO: Ask JO what he's doing with 3D and what KP recently OK'ed wrt 3D libraries, certificates, downloading separate packages, etc.

CM TODO: Investigate 3D solutions for molecule with translucent electrostatic potential representation (electrostatic potential view), OR translucent shape where saturation of blue varies (electron density view).

Interviews deadline: Fall 2011