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
Mockup
Online Resources
Teaching Ideas
Interview Feedback
Discussion
Website

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?*

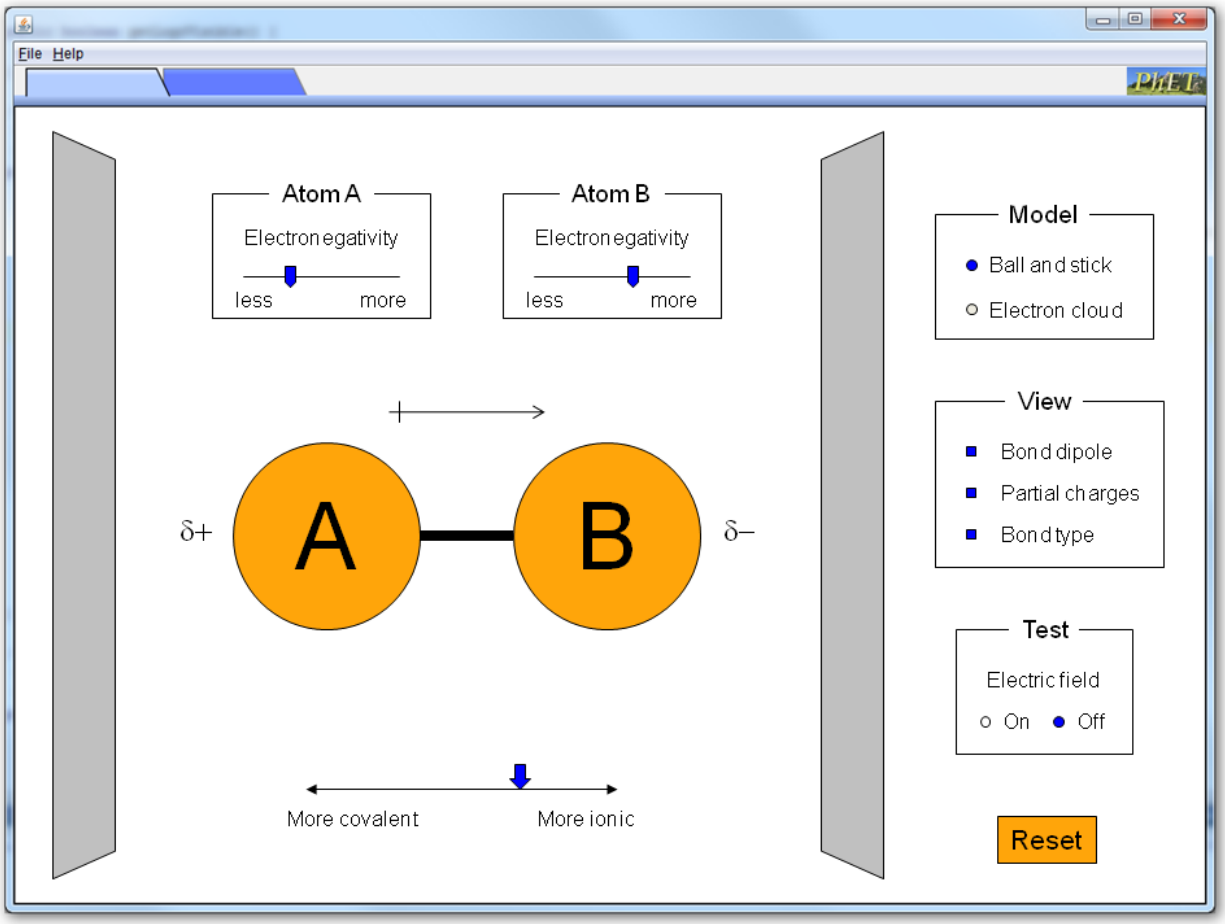
a. If each A has 2 lone pairs and Z has no lone pairs.
b. If Z has 2 lone pairs and each A has no lone pairs.
c. If Z has 1 lone pair and each A has 3 lone pairs.
d. If A is drastically more electronegative than Z.
e. If Z is drastically more electronegative than A.

	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)**

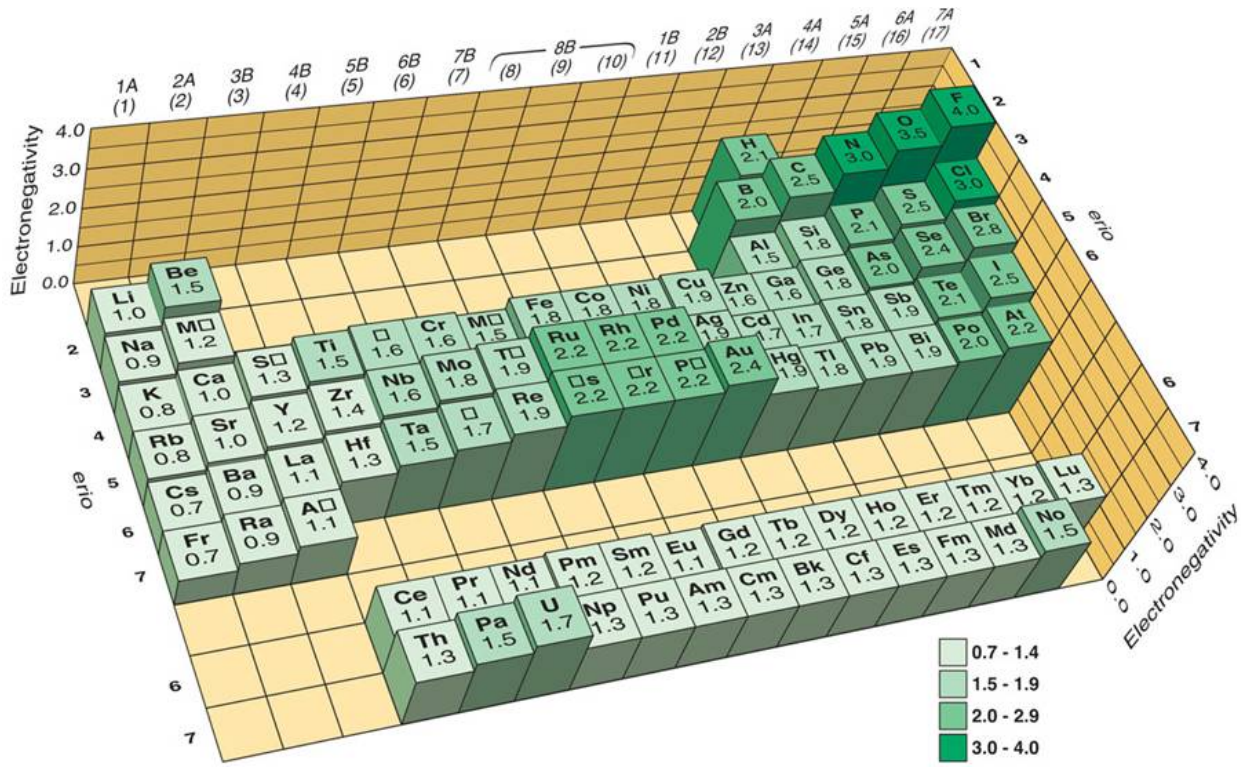
Mockup

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

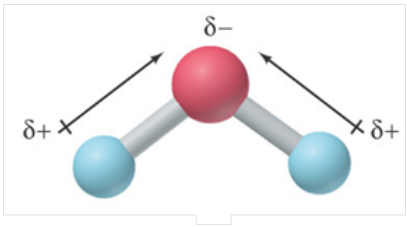


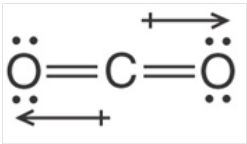
<u>Change electronegativity</u>
Students can use a slider to change the EN of each atom. EN is the ability of a bonded atom to attract the shared electrons. Below is a chart of relative EN values. The max value is 4.0; the min value is 0.7. Should the slider go to zero? Should we show the EN values?
Update: snap to tick marks

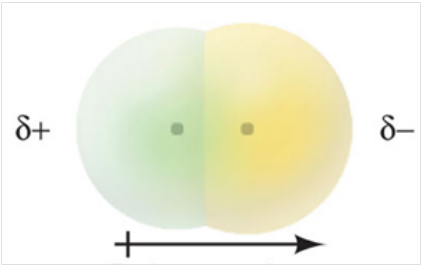


<u>Show bond dipoles</u>

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.

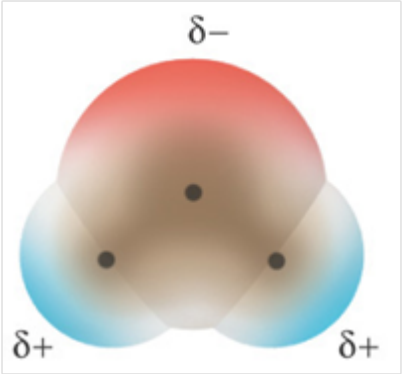
CM: I’ll be really surprised if “using the sim” leads to the conclusion that the cross at the arrow tail means “positive” and the arrow head is therefore negative.

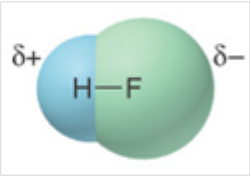
KL: By interacting with the sim, and changing the polarity, I think students will develop a working definition for the bond dipole (and the arrow that represents it).

<u>Show charges</u>

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.





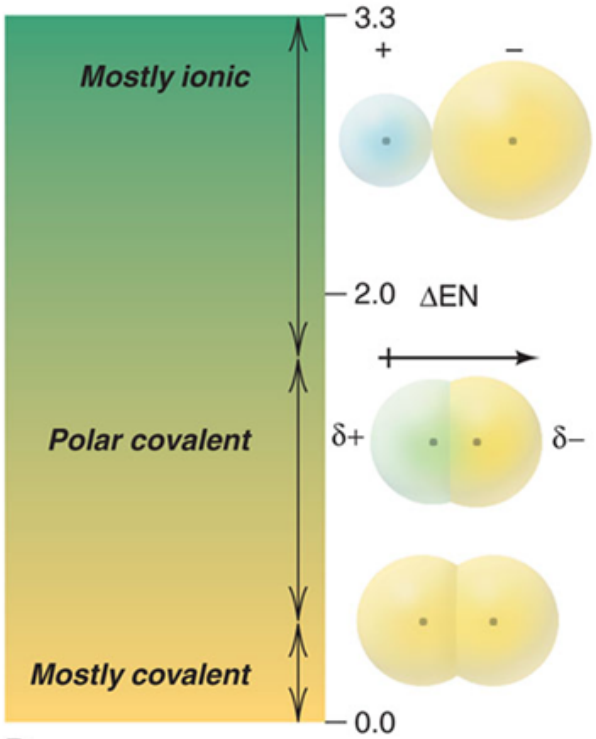
CM: Is the student expected to know these representations for charge?
KL: Is your concern with the delta symbol?
CM: Yes, concern is with the delta. Who is the audience? (I don’t see that in this doc.) Will they be familiar with Greek characters, know that this is delta, and know that delta means difference? 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

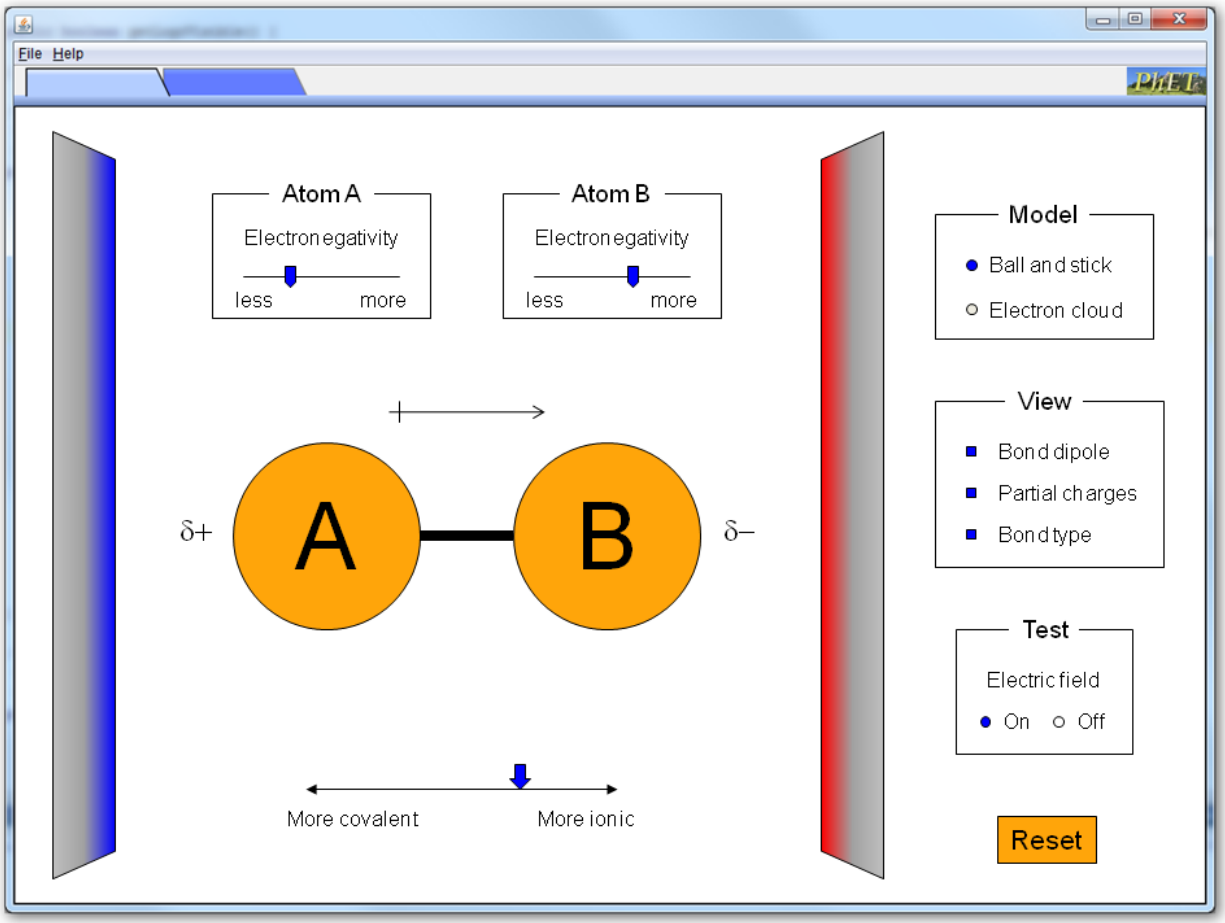
Show bond type
A dial shows if the compound is “more ionic” or “more covalent.”

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

A

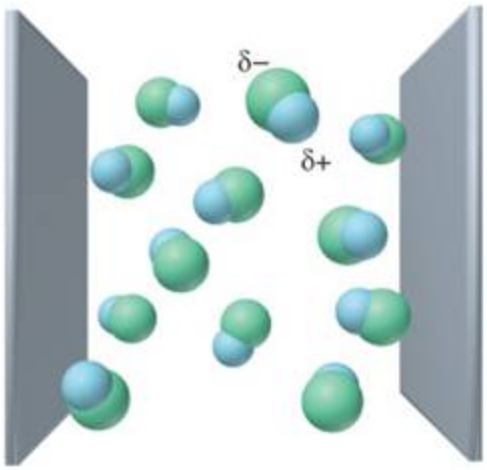


B

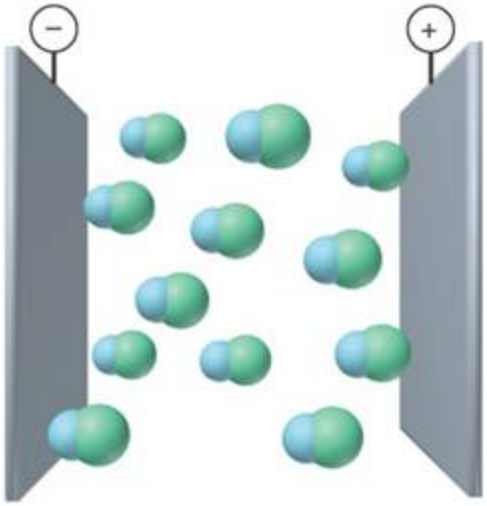


<u>Electric field off/on</u>

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

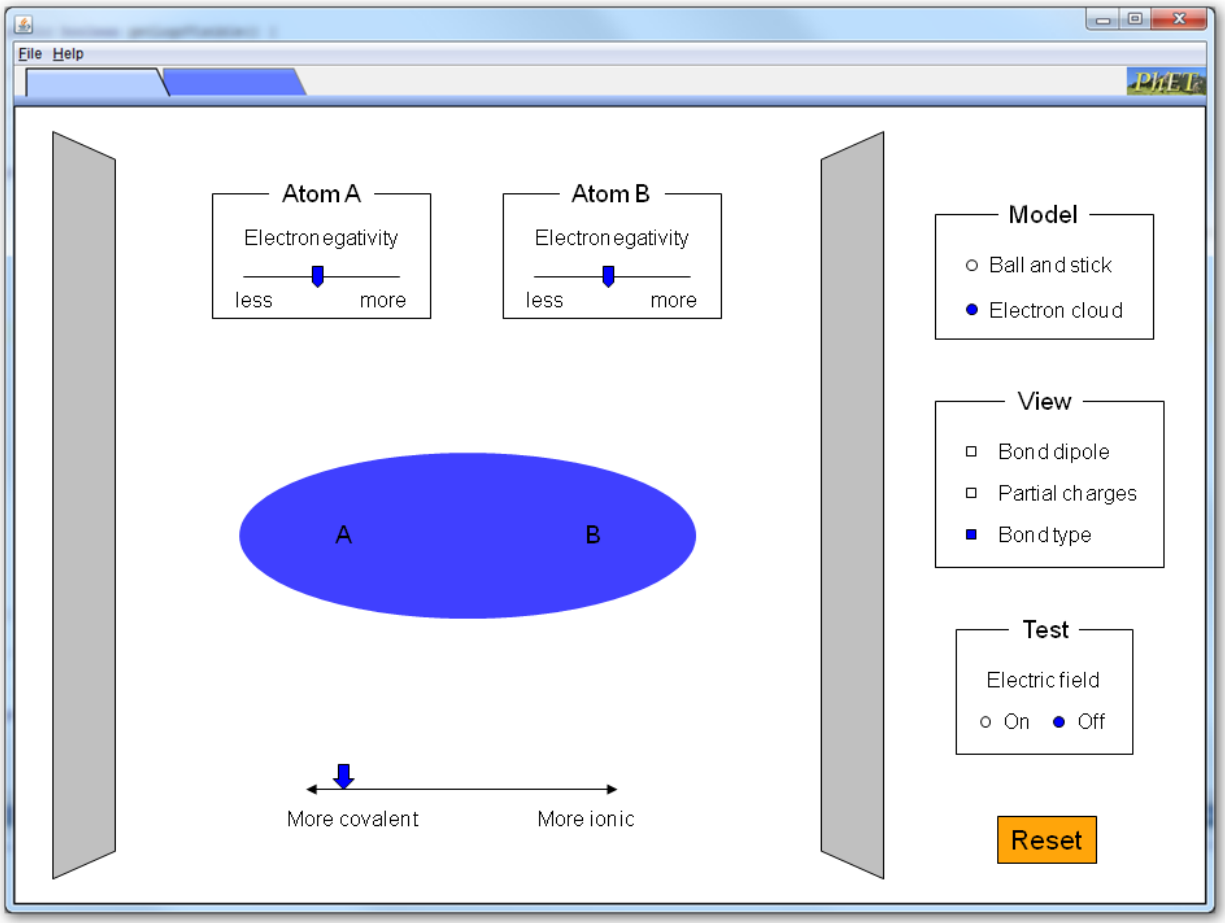


B Electric field off



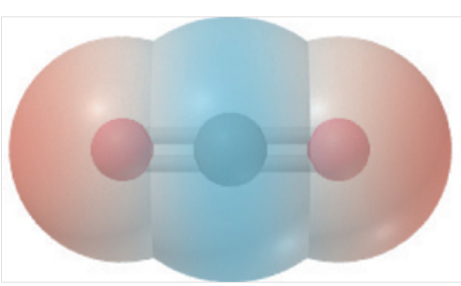
C Electric field on

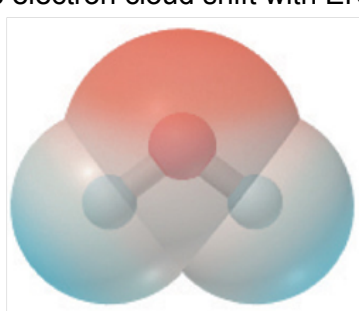
CM: Should the plates be labeled positive (+) and negative (-)? Why is only part of each plate colored? Is charge only on the back third of the plate?
KL: Yes, the plates should be labeled, and no, the charge is on the entire plate. The color is an attempt to give students another visual indicator that 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.



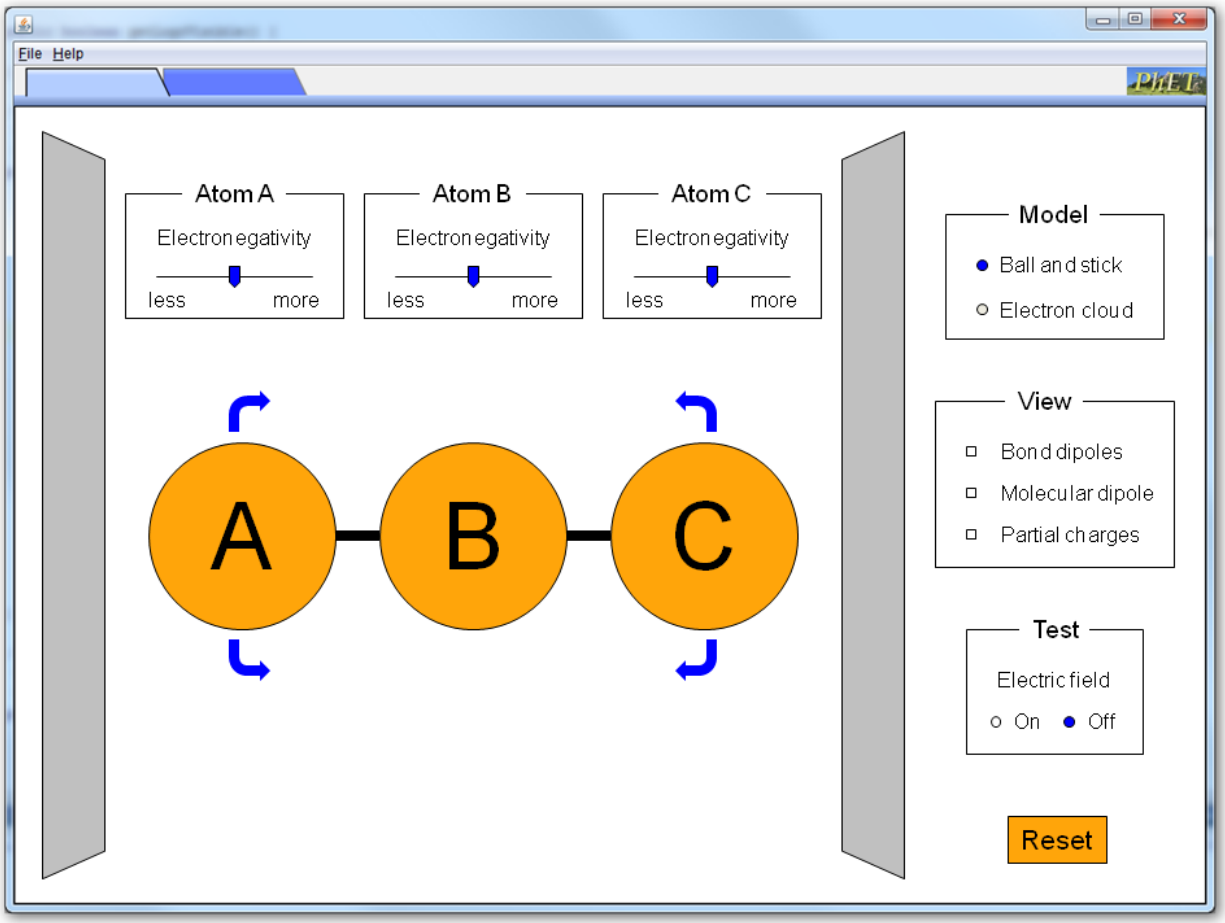
<u>Show electron density</u>

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!



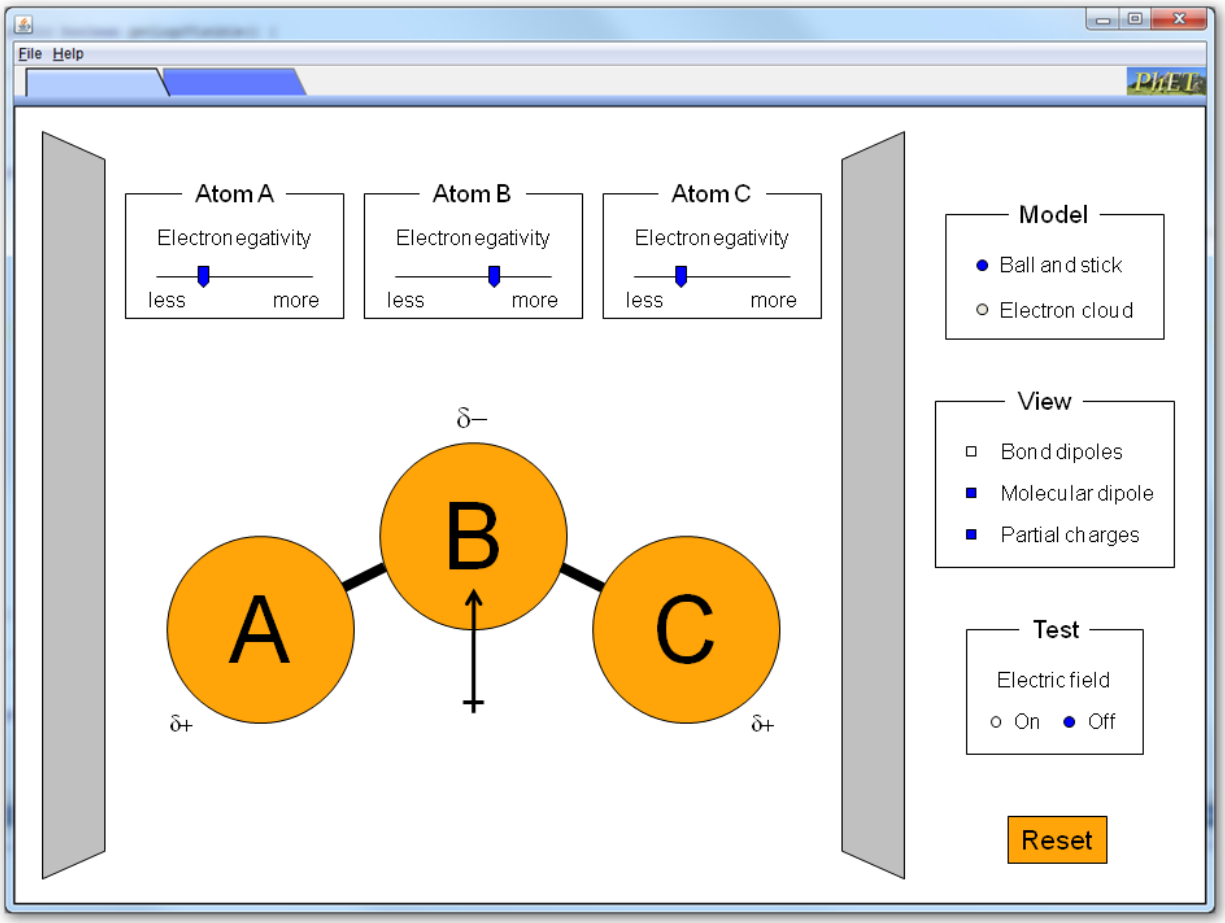


Tab Two: 3-atom molecules



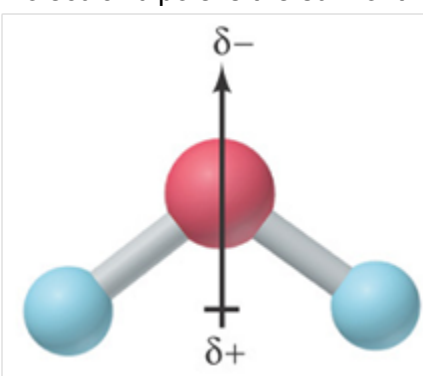
<u>Change shape (or angle)</u>
Two ideas: 1) students can interact with the atoms directly, or 2) students can use a slider that changes the angle. Try option one first. The bond *length* should not change.

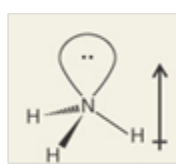
CM: What do the blue arrows mean?
KL: The arrows are not visible to students, they are meant to indicate that students can drag the outer atoms up or down.
CM: OK, I see... they are drag handles to change the angle. I think we should change the cursor to this type of arrow on mouseover.



<u>Show molecular dipoles</u>

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.





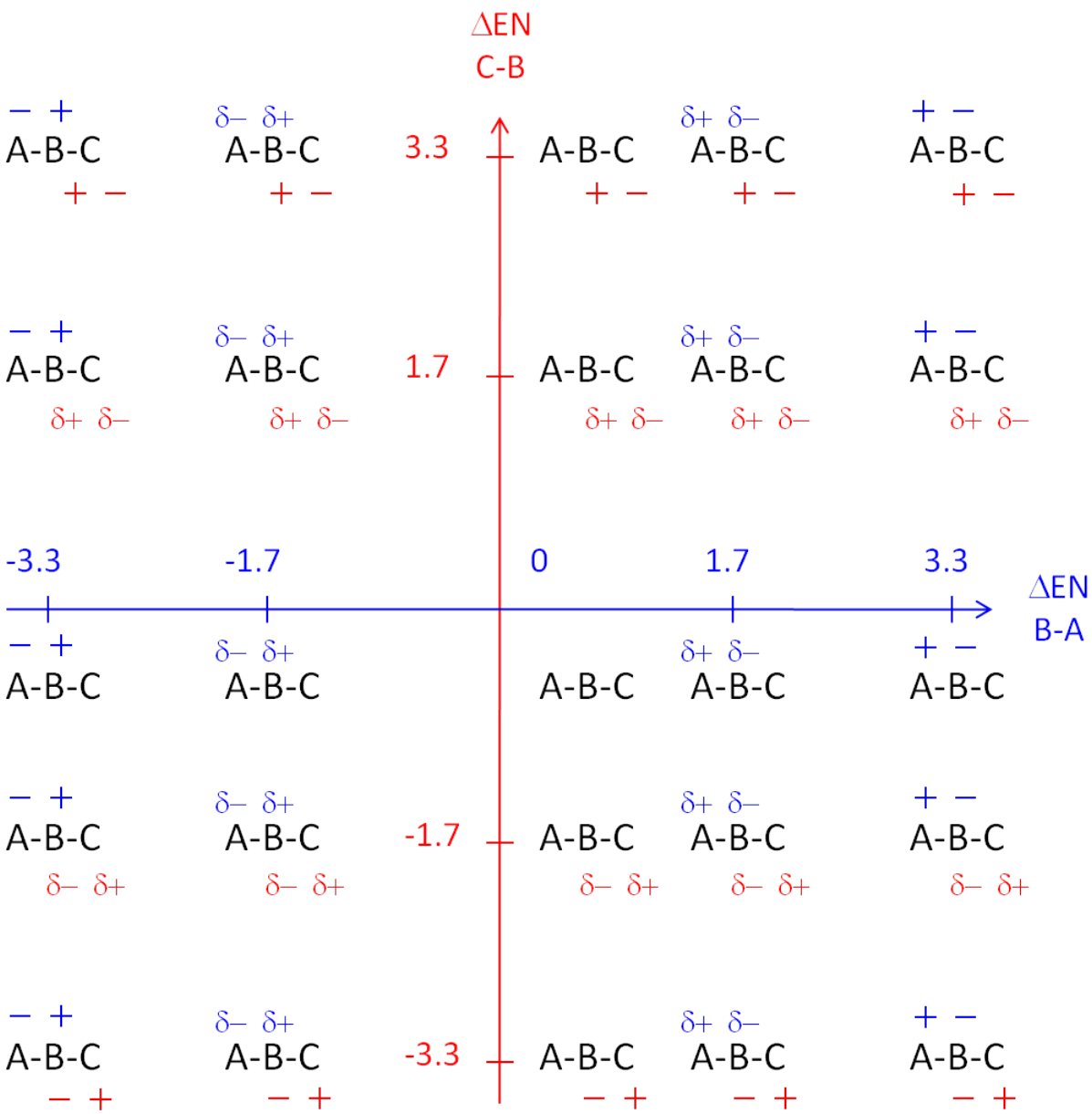
CM: Bond dipoles and molecular dipoles use the same representation. Do these View options need to be mutually exclusive? (radio buttons instead of check boxes)

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.

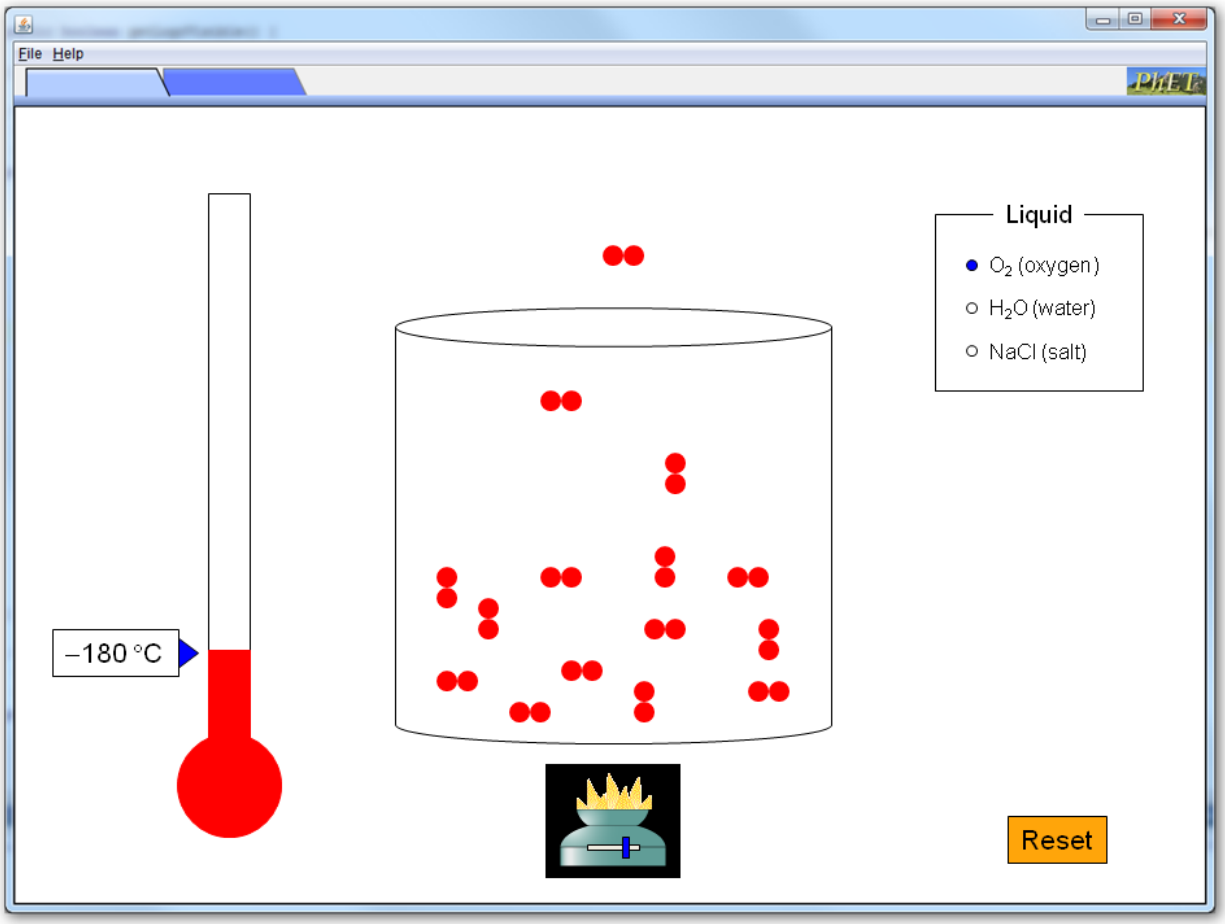
Model
- need to convert EN difference to partial charge; fine for 2-atom case, but 3-atom case is complicated
- could treat A-B and B-C independently (see below), but need to consider 3-atom interaction to account for the polarity of O3
- can get ionic and covalent bonds in same molecule; could limit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



Tab Three: Real molecules

Need to mockup!

Tab Four? Boiling Point



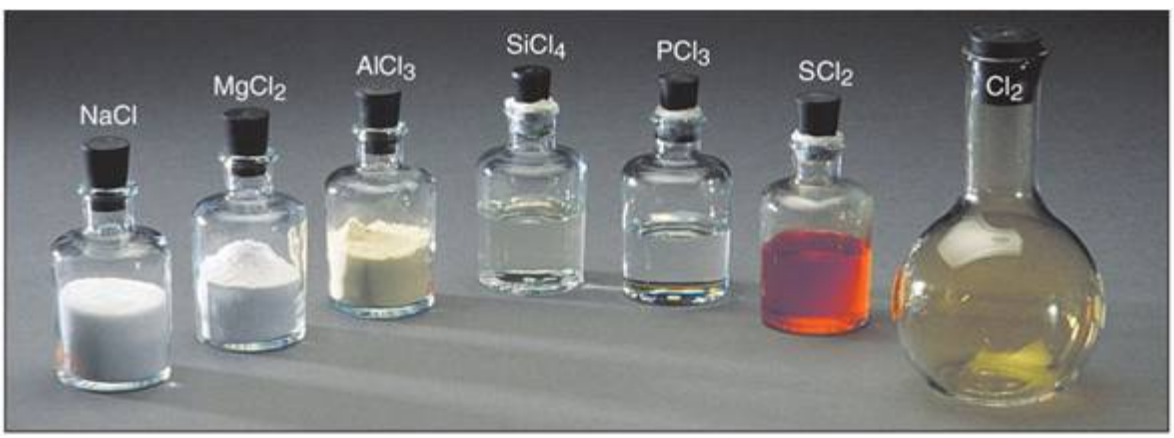
<u>Measure boiling point</u>
Students can add heat and see a liquid become gas. See the [States of Matter] sim for an example. They can measure the BP with a thermometer (default units = C). Below is a table of melting and boiling points.

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.

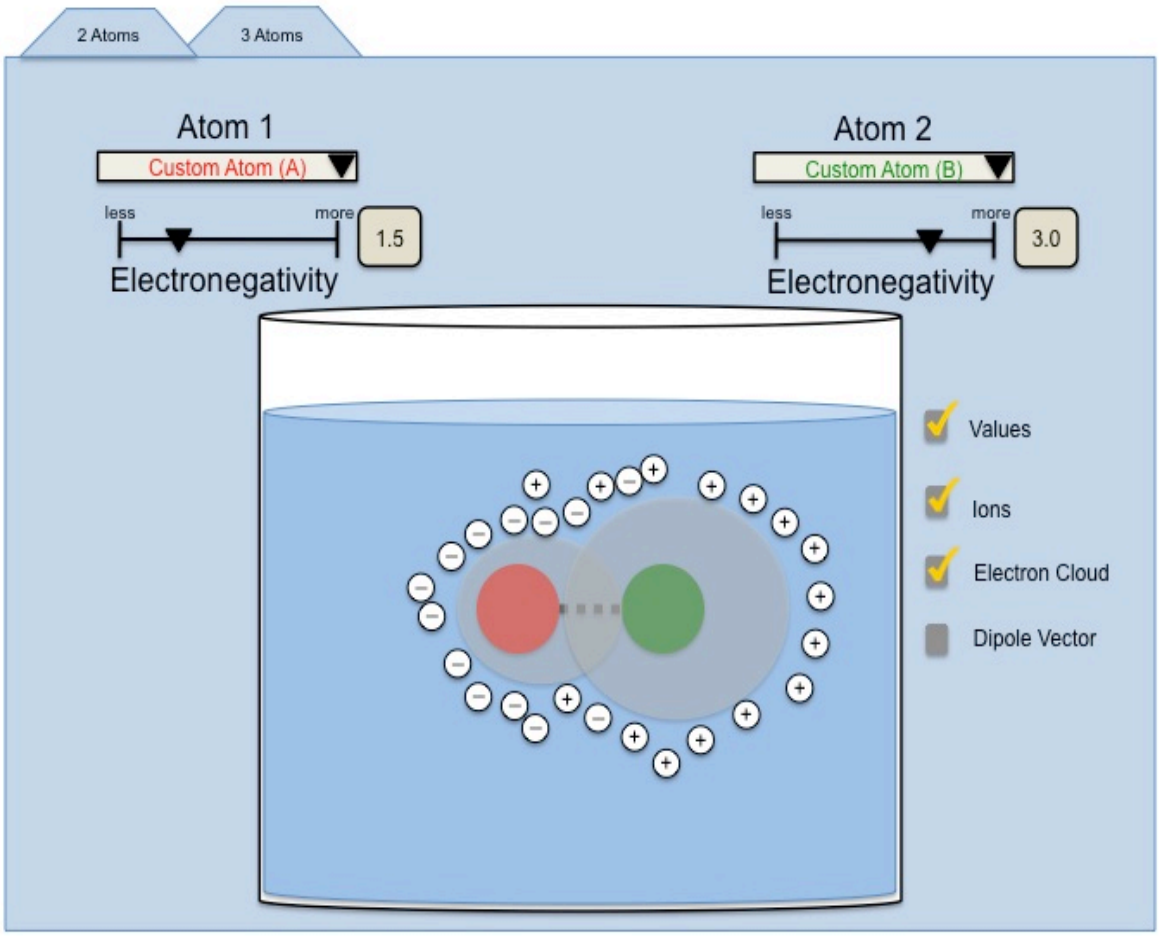
Polarity

- 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

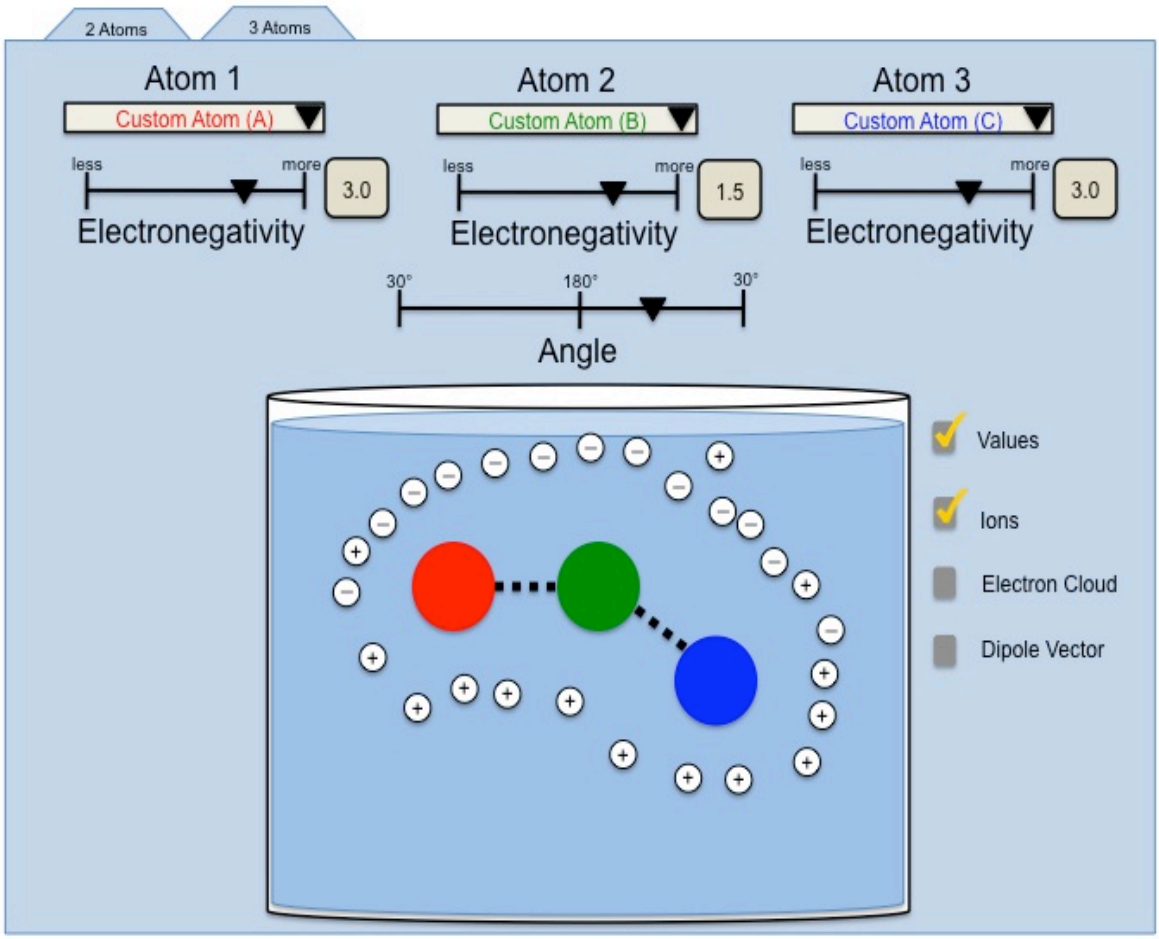
- each atom has its own slider which controls electronegativity
- separate slider controls angle between the three atoms
    - default = 180°, range = +/- 30°

- 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

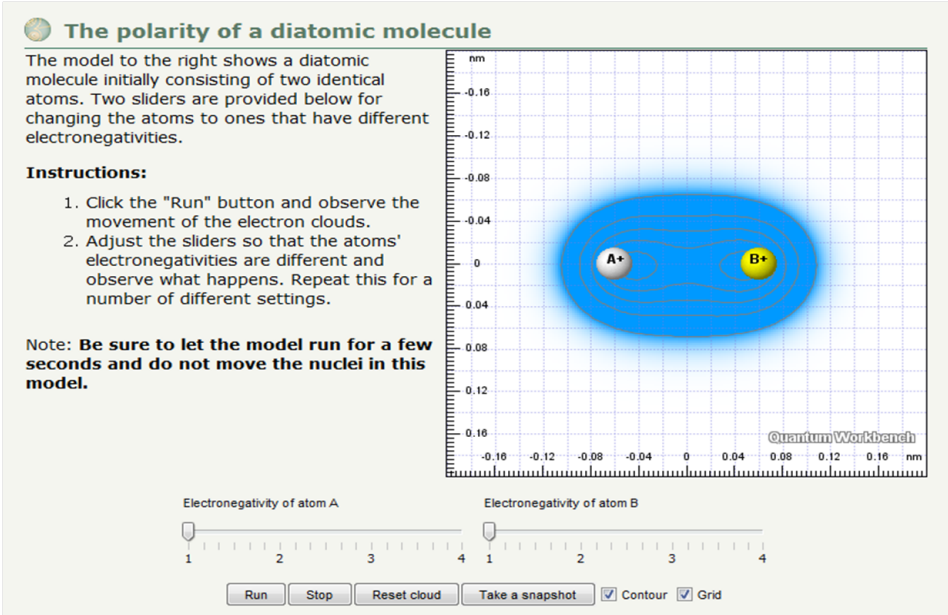


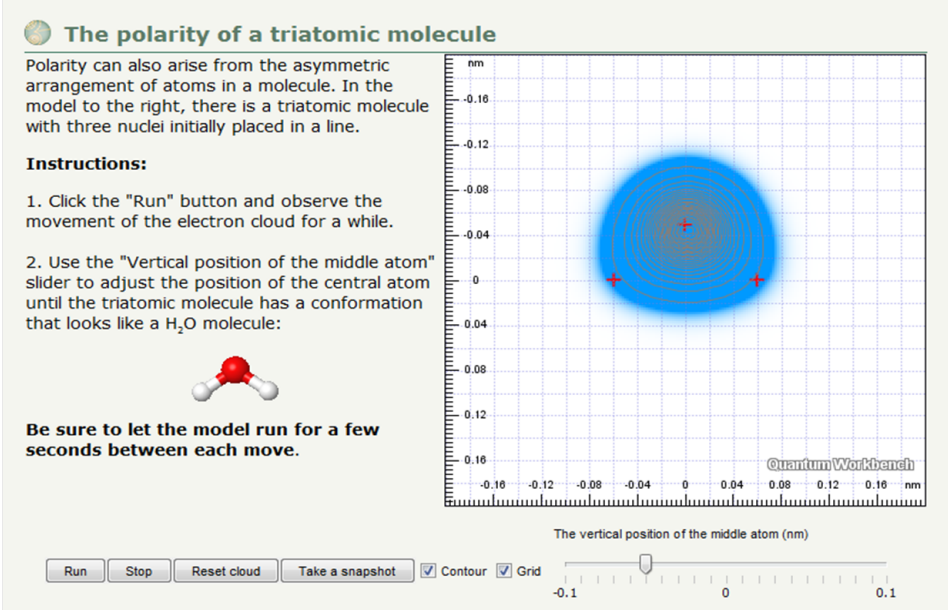
Online Resources

Wikipedia article on chemical polarity.

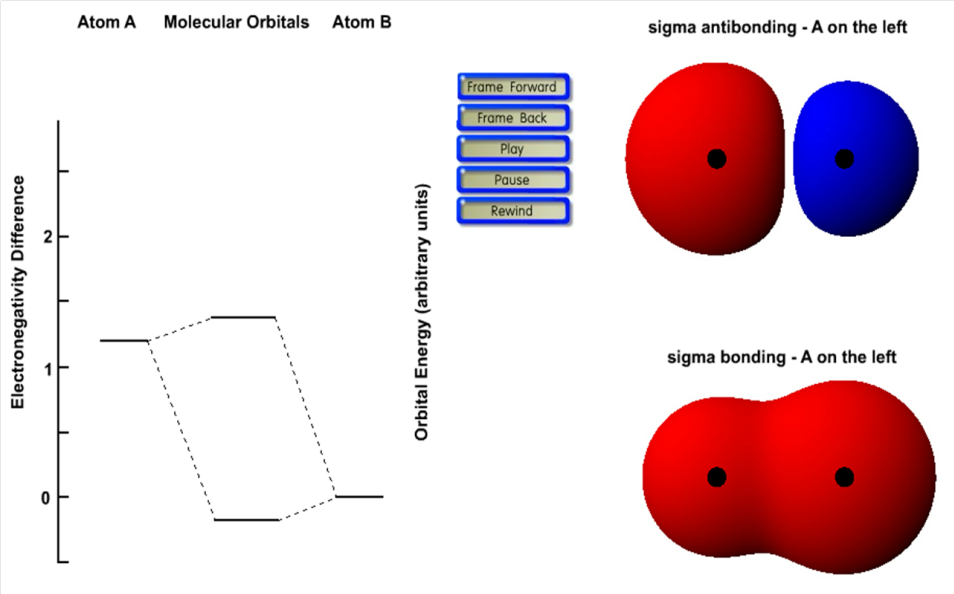
Other Sims

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.

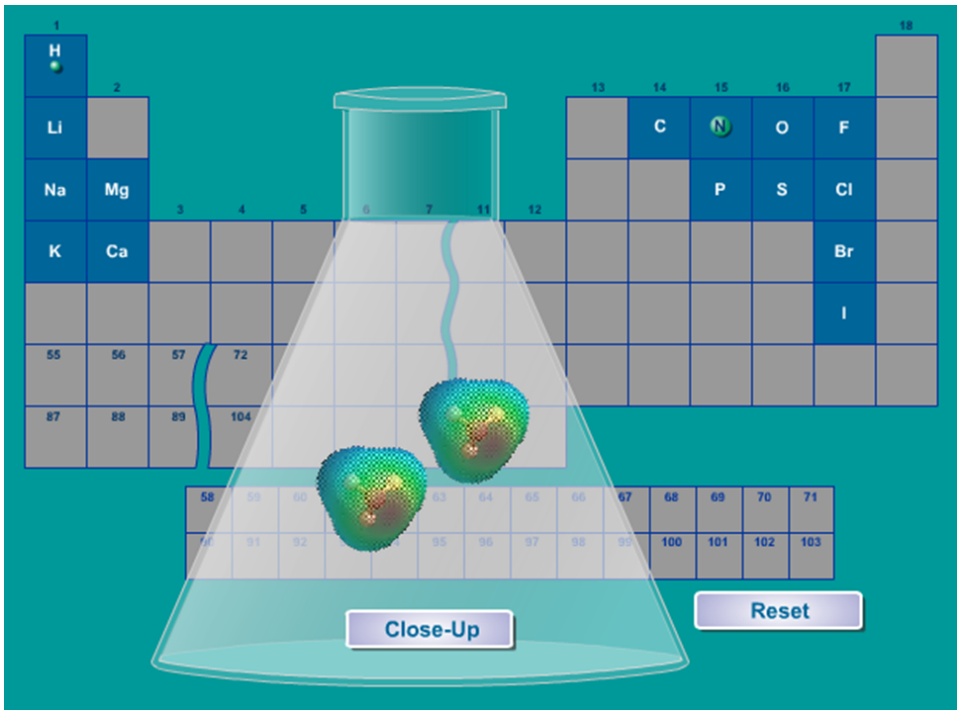




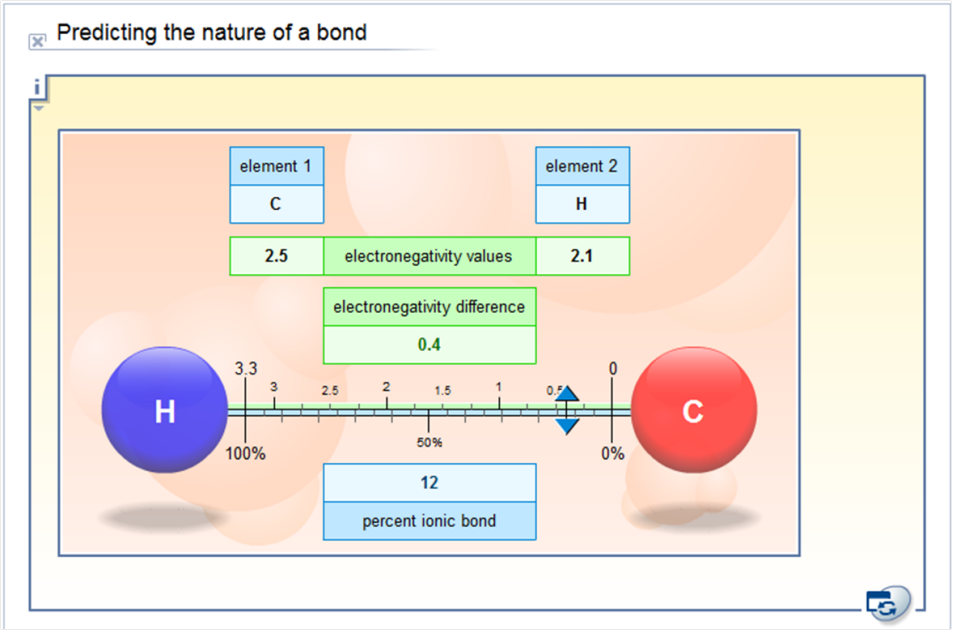
KL: This animation was shown in a talk at the GRC:
http://www.wellesley.edu/Chemistry/Flick/chem341/mocovtoionic2.html



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

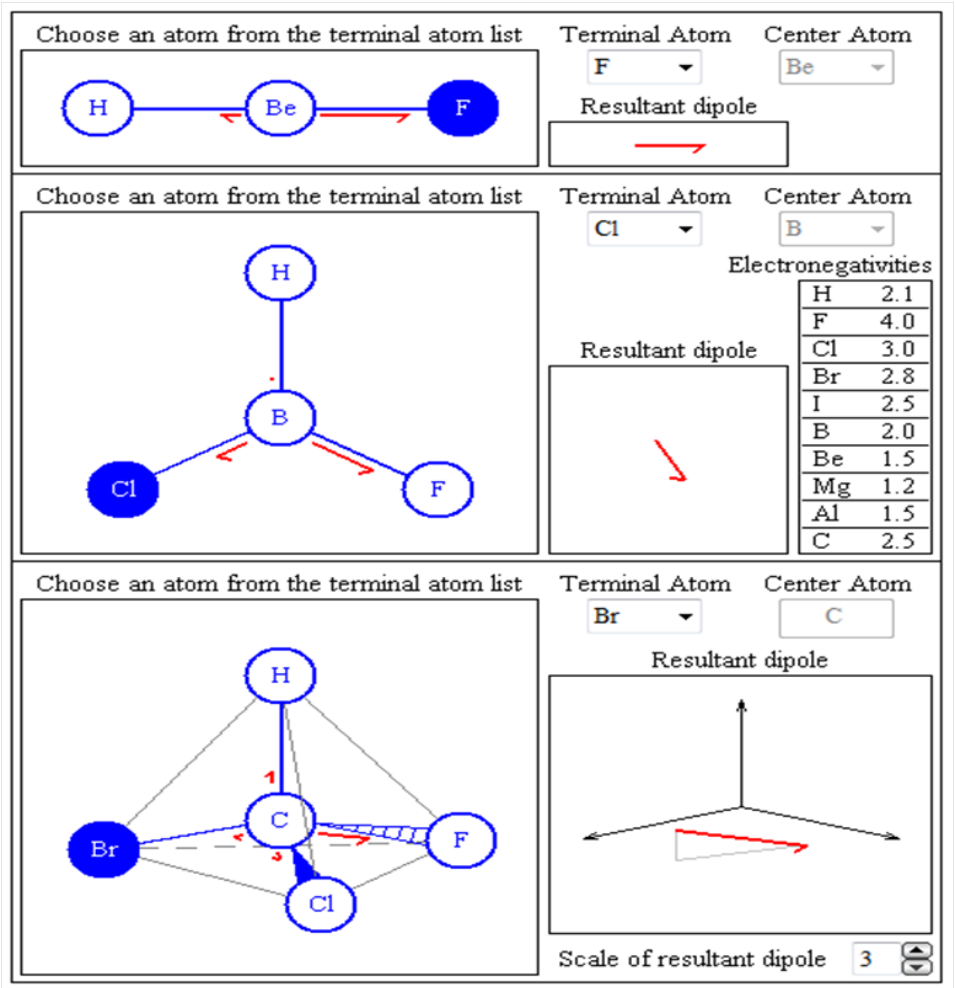


http://www.yteach.co.uk/index.php/resources/electronegativity_polarity_variation_periodic_table_group_bond_t.html



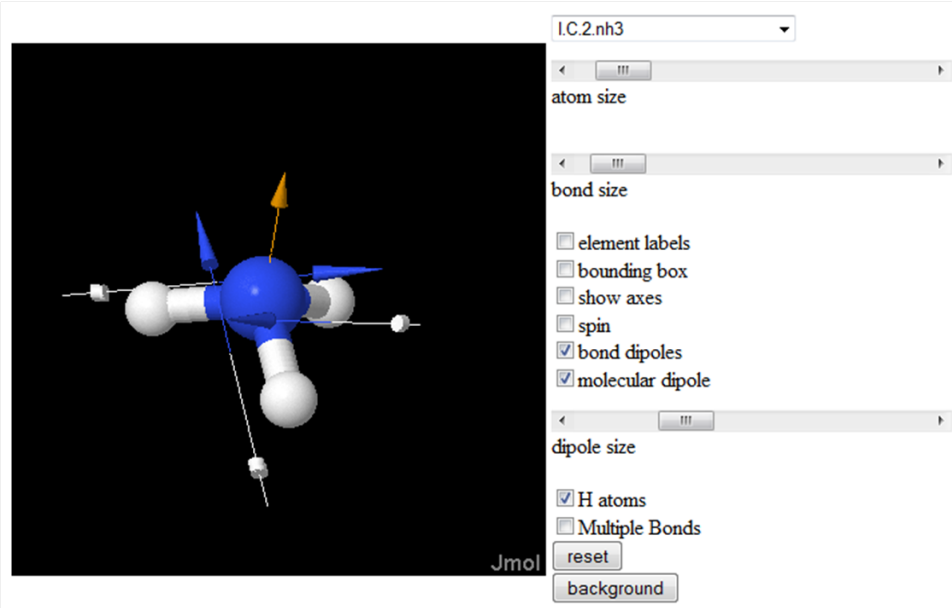
JC: I tried the above sim; it seems like a useful tool (you have to enter numbers, no dragging sliders) but after one use I got a big “You must buy a licence” message. If/when you try it out, observe as much as you can on your first use.

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.

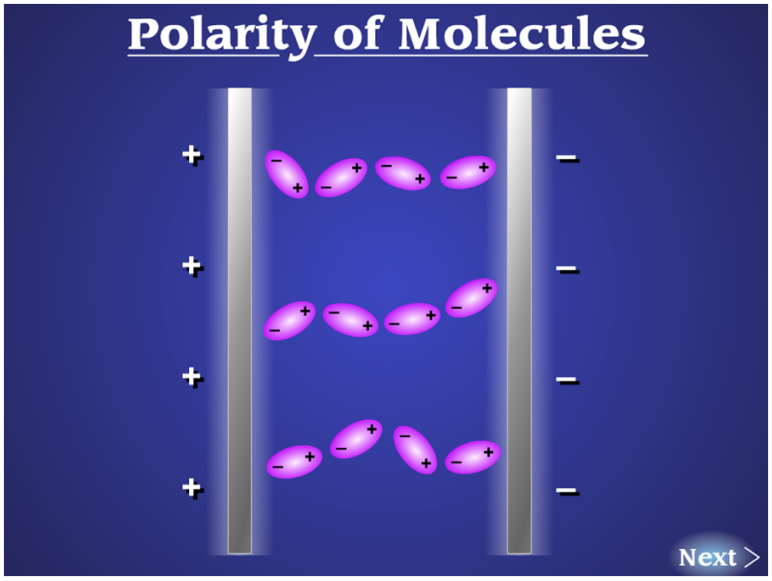
CM: Wow, that really is a horrible user interface. It looks like there are some bugs in the molecule rotation algorithm, too. Shouldn't be too hard to do better than this.

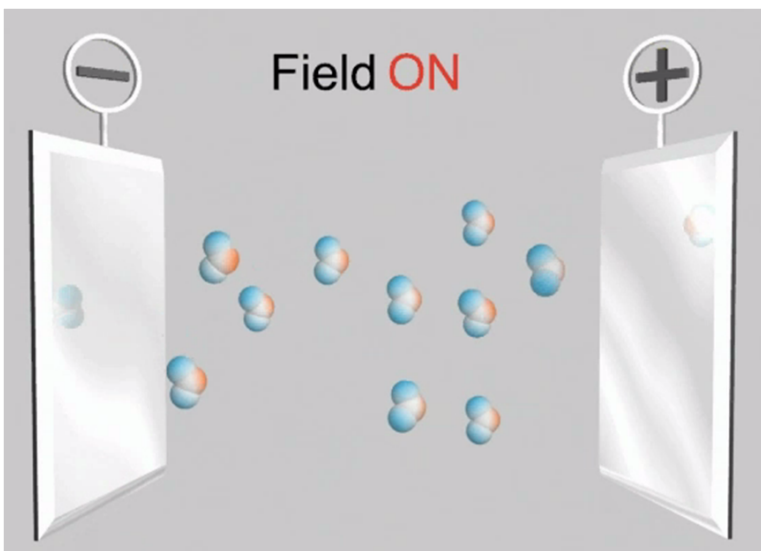
CM: Here's a page that "illustrates the new capabilities of Jmol to calculate and display dipoles and simple arrows."
http://chemapps.stolaf.edu/jmol/docs/examples-11/dipole.htm

JC: Here is another link to a free molecular modeling software program for visualization. This is probably more powerful than we would need (it does protein ribbons!) but it could serve as a reference for checking (or assigning colors to) our electrostatic potential maps. I have not tried it out yet; we can discuss if we think it would be worth the time to do so.
http://www.arguslab.com/index.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

KP: Thesis on bond polarity and molecule shape:
https://mospace.umsystem.edu/xmlui/bitstream/handle/10355/4829/research.pdf?sequence=3

Teaching Ideas

We plan to use this sim in Susan’s gen chem class the week of 11/07/11

Interview Feedback

Protocol: (copy)
Post-questions: (copy)

S1M
09/09/11 v 0.00.19

Warm-up:
- soph, mechanical engineering
- took: IB chem in HS, intro chem at CU
- used PhET in HS (circuits)

Sim:
1st tab (3 mins)
uses EN sliders, then checkboxes
on bond type, uses sliders
clicks back & forth btwn surfaces
stays on ED, uses sliders
turns on E-field, sees no align
uses sliders, sees align
2nd tab (3 mins)
uses EN sliders, all checkboxes
asks: what do bond dipoles represent? direction of force?
turns on E-field, sees align
3rd tab (30 mins)
looks at menu, checks all views
tries to remember PT trend for EN
selects NH3 (all views on, then turns some off)
says it (MD) comes straight out
selects H2O, **rotates**, turns on surface

says arrows are lone pair electrons
stays on EP surface, selects H2, HF, N2
says not sure what MD is showing
says maybe (none) b/c 2 similar atoms
turns views off/on, selects F2
says when diatomic molecule, partial charge is 0, no EP or electron density
selects diff molecules, looks at charges
rotates when not aligned well
says atoms w/ higher EN have neg partial charges
says EP follows where neg PC is
selects ED, says also follows w/ neg PC
picks O3, turns off surface, checks dipole
(back to 2nd tab)
rotates the molecule
(back to 3rd tab)
says it sort of matches (O3 & 3-atom)
says wait a second, this has the same...
says here (3rd tab) all have same EN (uses mouse to indicate bond dipole)
says here (2nd tab), if have same EN, dipoles disappear
says but they don't have same partial charge (in 3rd tab)
turns on MD, selects diff molecules
says bond dipoles start at lower EN, go to higher EN
says molecular dipole = net sum of bond dipoles
says bond dipole goes from C to F, MD is sum of those
says BD go from high charge to low charge
says here (BH3) it makes sense that no MD; all cancel out
(in 2nd tab)
tries to match H2O w/ 3-atom tab
says partial charge depends on atoms
says for O2, same EN, PC=0
says for CO2, diff partial charge b/c C is there
selects CHCl3, says can't see, but assume dipoles go from C to Cl
turns on both surfaces
selects CH2O, tries to **predict** bond dipoles
says for this section (points w/ mouse), MD down, for this section, MD up
so predicts that MD goes up (checks)
says no trend w/ partial charge & EN
says maybe has to do w/ structure
says no correlation btwn EN & partial charge
<u>Other</u>
KL: think?
says nice if had full PT to see trends
says if had just learned in class, would be helpful; not something to look at first
KL: learn?

says refresher about dipoles, how lone pairs affect structure
says nice if water had lone pairs, to know it's there
KL: surfaces?
ED is more self-explanatory: more electrons on this side
EP is same: more neg here, neutral in middle, pos on this side
says size of circles is arbitrary
KL: change EN?
says no option in 3rd tab
says each element has it's own EN
when slide, it changes identity of atom

Follow-up:
all correct, but did not put delta symbol in front of charges

Notes
- spent way more time on 3rd tab (30 mins) than 1st and 2nd tabs (3 mins each)
- did not rotate molecule in 1st tab, or change bond angle in 2nd tab
- said atoms w/ higher EN have neg partial charges
- noticed O3 has dipole, but in 2nd tab, if have same EN, no dipole
- said bond dipoles start at lower EN, go to higher EN; molecular dipole is net sum of bond dipoles
- tried to predict direction of dipole, then check w/ sim
- said no correlation btwn EN & partial charge; maybe has to do w/ structure
- said each element has it's own EN; when use slider, it changes identity of atom
- all correct on post, but did not put delta symbol in front of charges

S2F
09/09/11 v 0.00.19

Warm-up:
- junior, integrated physiology
- took intro chem at CU
- saw PhET in intro sim (acid-base)

Sim:
1st tab (6 mins)
says hard to talk out loud
clicks on molecule, does not rotate
uses EN sliders, views, EP surface
tries to drag bond type indicator
rotates molecule
turns on E-field, sees align
resets
says has not learned yet
says the arrow always goes to pos side (plate)
says colors represent pos or neg

says can still be pos or neg w/out E-field
says if no EN, does not matter if field on
says least EN atom always points toward neg plate
says moves slower w/ less strong EN
says if equal EN, don't move
says EN affects the bond type
says covalent if no charge
<u>2nd tab</u> (4 mins)
says it shows 3D axis
says not sure where arrow points; oh, to most EN
says no charge if no EN
turns on bond dipoles, partial charges
says more EN = neg charge
turns on E-field
says neg plate attracts pos "molecules"
says arrows point toward pos plate
says not sure what dipoles are (depoles)
<u>3rd tab</u> (7 mins)
clicks in menu
says shows diff molecules & bonding
rotates, shows dipoles
says MD does not do anything to that molecule
finds one w/ mol dipole
selects EP & ED surfaces
says more e-s where more EN
says EN even for all molecules w/ same element; same density, zero E-potential
says shows diff molecule shapes
selects O3, says hmm
says weird that shows blue & red even though same molecule (atom)
likes that it tells you name of molecule
says MD points toward more EN; or red or darker gray
looks at options menu, changes to rainbow
on CH4, says green, so mostly neutral
tries to find one that is not "even"
picks HF, says F more EN
goes back & forth btwn EP & ED
says EP shows neutral along bond
likes the rainbow
clicks help in menu
says you can make 2nd tab like real molecules
tries to make H2O
figures out can change shape
makes B like oxygen, other two (like H)
says can only move in 2D

says prob move slower if less EN; tests
says the bigger the greek letter, the more pos; same w/ black arrow
Other
KL: think?
says not sure about applications of it
says no idea what “depole” is
knew EN increases from left-to-right in PT
KL: learn?
says easier to understand EN if can mess with it
KL: change EN? says maybe
KL: surfaces?
says ED more clear; shows where more e-s, makes more neg on that side
says not sure if EP is diff; red is always on darker side
says more EN = more dense
KL: dipole?
says BD shows where pulling
says MD points toward more EN atom
says did not see at first, hidden for some molecules (NH3)

Follow-up:
played for about 25 mins
drew correct length & direction of bond dipoles, correct charges
did not understand molecular dipole

Notes
- played for about 25 mins
- noticed the molecule aligns w/ E-field slower (when dipole smaller), not at all if equal EN
- had never heard of dipole; said “depole”
- noticed that EP for O3 is blue & red even though same (atoms)
- used the options menu to change the colorscheme to rainbow
- figured out you can change angle in 2nd tab when she tried to make H2O
- said the bigger the “greek letter,” the more pos
- said ED shows more EN = more dense, more neg on that side
- on post, drew correct length & direction of bond dipoles, but did not understand molecular dipole

S3F
09/12/11 v 0.00.20

Warm-up:
- freshman, MCDB
- took AP chem in HS
- used PhET in HS physics (roller coaster)

Sim:
clicks tabs (in no order)
selects water from drop-down

says looking at polar molecules
clicks views, says diff ways it can be shown
uses EN sliders (1st tab)
says when you increase EN, it shows dipole
says it shows diff charges, etc.
says it starts basic, then 3-atom, then real
(after 4 mins) asks: is that all?
says it shows which way charges/dipoles go
says real shows exact charges, common diatomic molecules, etc.
says maybe talk more about surfaces
(after 2 more mins) says that's it
says doing in lab right now
rotates the molecule (1st tab)
tries to drag bond type readout; says not sure what it's showing
says maybe about bond in middle
says covalent & ionic bonding are diff
uses EN slider, says oh!
turns E-field on, says it helps understand concept
likes the key, PT (3rd tab)
says confusing to have them all clicked
on HCN, says not sure about MD
picks diff molecule, says oh, it's an arrow
(after 7 more mins) asks if more
likes that starts basic, goes to real
says does not show bond type (2nd tab)
says not sure about surfaces
says EP shows more pos/neg
says as you change EN, gets more dense on one side
says E-field shows it attracts/repels
says more EN = attracted to pos side
says charges help understand shape
says it shows dipole points from pos to neg
says I guess MD is overall direction & shape
says EP surface shows neg & pos
says it shows where other molecules would bind!
says for ED, more = darker
says it shows where more electrons; maybe valence?
says it looks the same for diatomics, could relate (1st and 3rd tabs)
resets
<u>Other</u>
KL: bond angle?
says if both same (EN), do same thing
talks about A & C repelling each other
KL: rotate 3D?

says it helps show shape, where the bonds are
KL: surface?
says EP more helpful, about charges & dipole
says not sure how ED affected by charges
KL: change EN?
says not in real life
says it shows what kind of bonding would happen

Follow-up:
used sim for about 20 mins
on Q1, gets dipole backward; says more EN = pos charge
on Q2, gets dipoles correct, but says polar
for part 2, says nonpolar, draws interesting shape

Notes
- not in learning mode; after 4 mins, asked: is that all?
- did not change bond angles or rotate in 3D
- said it starts basic, then 3-atom, then real
- confused by the bond type indicator; tried to drag
- said EP surface shows pos & neg, where other molecules would bind
- said ED shows where more electrons
- talked about atoms repelling each other
- on post, got some ideas backward; said more EN = pos charge
- showed Molecule Shapes at end of interview

S4M
09/12/11 v 0.00.20
(JC observed)

Warm-up:
- freshman, physics & molecular bio
- took regular chem in HS
- never used PhET

Sim:
1st tab (4 mins)
uses EN sliders
says it switches, disappears
clicks partial charge, not sure about symbol
uses EN slider w/ bond type
gets it to go all the way to ionic
clicks EP, uses sliders
says it becomes more neutral/more polar
turns on E-field, did not align!
2nd tab (4 mins)
rotates molecule
says if make more EN, charge goes toward it

turns on E-field, sees align!
says when more EN, attracted to pos plate
(back to 1st tab to rotate molecule)
says more EN attracted to pos
says can see ED, more e-s on this side
says EP shows polarity
<u>3rd tab</u> (20 mins)
rotates in 3D
likes diff atom sizes
(back to 2nd tab to check)
says arrow means more neg on that side
says yep, charges say neg
says the more I add on (views), the more I see that's neg side
tries H2; says it's neutral, no charge
says all these neutral b/c same atoms
picks water: says O neg, H's both pos
on ED, says most e-s on that side
picks CO2: says looks symmetrical, shows bonds
resets, says oops
picks HCN: says dipole goes off "map"
says it shows in 3 diff ways, where e-s are & the charges
says it shows charge relations & EN
picks NH3, says more complicated
says all H's are being pulled toward center
likes that it shows shape of bonds
picks BH3, says less extreme charge, so less color
says EN chart helps make sense, can get overwhelming
says big arrow is overall polarity
picks CH4, says hard to imagine if could not rotate
says charge diff not big
uses middle mouse to **zoom** in!
says you can use to test yourself: guess the charge, etc.
says EN chart is cheat sheet
picks more complex molecules, says never heard of before
on CHF3: says all F's are neg, H is pos
says fun to play around with
says names are kinda intimidating
on CF4: says looks even, more dispersed
says all charges cancel out, so it's stable
says makes a lot more sense now
(back to 1st tab)
says if increase EN, get stronger
says if both really EN, no bond (?)
says he wants E-field on 3rd tab

(on 2nd tab) says can make it rotate like a clock
changes to rainbow option!
says more precise, shows whole spectrum
says he's done
asks if able to type in molecules (3rd tab)
Other
KL: change angle?
if put EN sliders in center, does not matter
KL: surfaces?
says ED seems redundant
says EP shows neg/pos, likes color (rainbow)
says red always goes toward pos plate
says more EN = attracted to pos
KL: change EN?
says no, no options to change (in 3rd tab)
says can make 1st tab like HF
says in real atoms, depends on how it's bonded
says as I change, it becomes a diff molecule (in 1st tab)

Follow-up:
played for about 30 mins
on Q1, correct signs, but used 2-sided arrow, not sure how to get exact charge
on Q2, drew surface, correct signs, not sure how to draw bond dipoles

Notes
- played for about 30 mins, most time on 3rd tab
- did not change bond angle
- said EP surface shows pos & neg, less color when charge diff not big
- said all these (H2, F2, etc.) neutral b/c same atoms
- used middle mouse to zoom in/out on real molecules
- said all charges cancel out
- said you can use the sim to test yourself: guess the charge, etc.
- changed to rainbow option
- said if you change EN, it becomes a diff molecule
- on post, got all charge signs correct, not sure how to draw bond dipoles

S5M
09/20/11 v 0.00.24

Warm-up:
- freshman, e-bio
- took regular HS chem
- never used PhET

Sim:
1st tab (3 mins)
says changes EN, says it reverses polarity

says B in middle, if go past, A becomes neg
says same should cancel out, (tests) says yep
says this should be the most (opposite ends)
clicks PC, uses EN sliders, says remembers “delta”
clicks EP surface, sees rotate icon (rotates)
says same as charge, but in color; maybe surrounding e-s
clicks ED surface, says it shows A has more e-s; uses EN slider, nods
turns on E-field, (no align), rotates
says opposites attract, so not going to stay (predicts)
says ok, even when slight, still fully rotates
says this (opposite ends) rotates fastest (predicts)
<u>2nd tab</u> (4 mins)
says B has all EN right now, everything polar
uses EN slider, turns on E-field
makes all same EN, **changes angle** (by accident at first?)
turns on bond dipoles, PCs, rotates, uses EN sliders
makes it linear, turns on E-field
says trying to see what happens if make it straight w/ charge (4:38-5:04)
makes all same EN, says nothing
says (A&C) should repel each other, would not stay like that; mentions “VSEPR diagrams”
<u>3rd tab</u> (20 mins)
clicks checkboxes, rotates, clicks EP surface
says thinks it’s ionic bonding b/c 1.7 diff in ENs
on N2, says even, covalent; clicks PC, nods
says O2 will be same (checks)
says it shows bonding, how many e-s it has
on H2O, says like 3-atom tab
says as a whole, dipole is pos that way, neg that way (gestures w/ mouse)
on CO2, says no overall charge; says lot less than that was (H2O)
on HCN, says “cool one”
says overall, charge is that way (gestures), even though linear
on ED surface, says like staircase
on O3, says that’s weird; all 3 O’s the same, but still has partial charges
on NH3, says should be neg (predicts), says yep; compares charges w/ H2O
on BH3, says polar covalent, but flat; says less than O3, which is weird
on BF3, says surprised not polar b/c F so EN
say no MD, prob b/c 3 of them, so cancels out
on CH2O, says O takes most of the e-s; says even C has pos charge
on CH4, says does not have one either b/c all cancel out
says all those (H charges) add up to that (C charge)
on CH3F, says prob same as CH2O, says yep
says less than formaldehyde b/c has extra H
says EP & ED surface always the same
on CH2F2, says weird one, so many diff atoms involved

says no dipole btwn C & H, little strange
says should be b/c diff charges, maybe dot means really small
on CHF_3, says pretty obvious; says C still takes up most of charge
on CF_4, says should not have any MD b/c 4 of them
on $CHCl_3$, says should be similar to CHF_3 (checks), says yep
says big bubbles for small charge
says dot must be small diff in charge; diff of 0.01 for CH_2F_2, diff of 0.02 for $CHCl_3$
says once you figure out trends, don't need labels
<u>Other</u>
back to other tabs, says likes how it builds up
picks HF, tries to make in 1st tab, says it's same thing
picks F_2, makes in 1st tab w/ EN sliders
picks H_2O, makes in 2nd tab
says wishes they (A&C) would repel each other
says 2nd tab doesn't have surface options
asks: any other things?
KL: learn?
says O_3, that those 2 (outer) carry charge diff than that (center)
says rest was refresher
says Cl below it (F) in PT, says CH_3F & CH_3Cl same structure
asks about dot in 3rd tab
says wishes you could zoom in, could see the arrow
again, says A&C do not "repulse"
KL: surface?
says talked about ED in HS, says more basic, explains EP
KL: change EN?
says no, all have their own set ENs (refers to sim)
says not a problem b/c atom "A"; can "play god" w/ ENs

Follow-up:
played for about 30 mins
got all questions correct

Notes
- played for about 30 mins, most time on 3rd tab
- made lots of predictions, used the sim to check
- changed angle in 2nd tab; made it linear to see if would align w/ E-field; wanted A&C to repel each other
- noticed O_3 is weird, all same atom but still polar
- said EP & ED surfaces are the same
- said "dot" must be small diff in charge; diff of 0.01 for CH_2F_2, diff of 0.02 for $CHCl_3$
- made "HF" and "F_2" in 2-atom tab and "H_2O" in 3-atom tab
- got all post questions correct

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)

<u>Title</u>
- RP: any PhET guidelines for this?
- Consensus: “Molecule Polarity”

<u>Cloud</u>
- 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

07/11/11 - Control panel

CM: What style of control panels do you want for Molecule Polarity?
Floating in the play area (ala Bending Light) or fixed along the right edge (ala Faraday)?
KL: I favor the floating panels, because I think the metal plates already define the play area, but I am open to your opinion: what do you think is best?

CM: I don't have a preference in this case. The controls shown on the right in the mockups are relatively general, don't really pertain to specific things in the play area, and they seem to work fine lined up along the right, so a docked control panel would work OK. But floating controls would be OK, too, just a little more expensive to implement since the support for them in phetcommon is less mature. If they're floating, there's probably no need to move them around.
KL: Ok, let's float.

CM: Okey dokey. You may see a couple of iterations with them docked until I get things working, faster that way.

07/12/11 - Switch

CM: Instead of a control panel with on/off radio buttons, how about a switch for turning the E-Field on/off?
And no, I don't think the switch needs to be labeled on/off.
Household switches aren't labeled, and somehow we all figure out how to turn the lights on.

KL: I do think it's a good idea to attach the E-field control to the plates, and I like your idea for a switch. Would it still be labeled as E-field? I think chemistry students may need the label to describe what they just turned on. (But no need to label on/off.)

07/13/11 - More 3D

- are diff reps ok? use same reps in 2D?
- CM will start on 1st & 3rd tabs

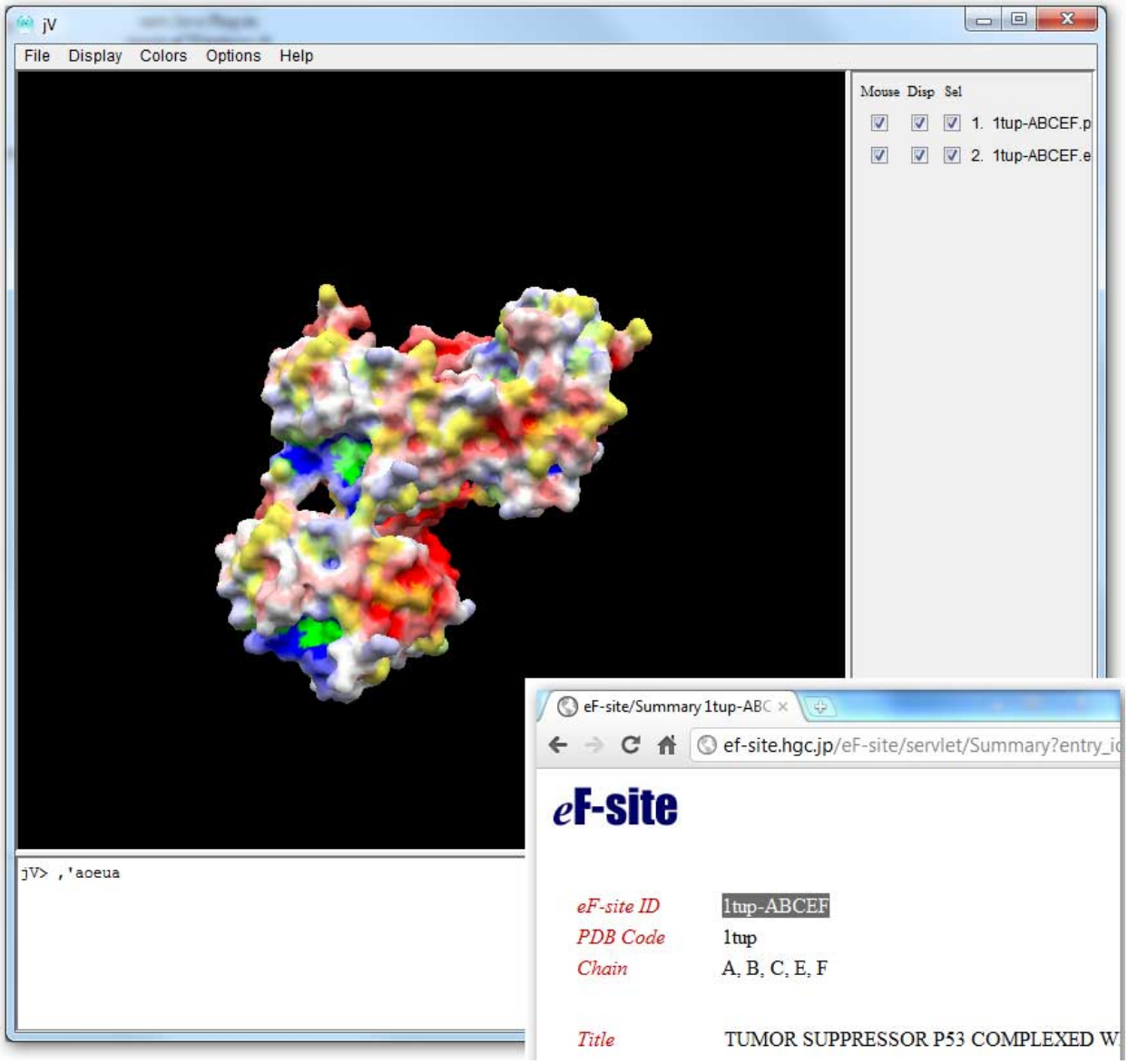
<u>Minutes from status meeting</u>
Molecule polarity. Going with floating control panels. KL talked about test thing. It turned the field on or off. These are going to be slanted with 3d perspective. At meeting last week had 3d requirements come up.
JMOL demo. Dipole feature. And also has translucent electrostatic surface. Haven't explored to see if it has other view that we made up. It is not a standard. KL: KP's idea "electron density"

And that view would be basically a single color, more saturated depending on where electrons are.

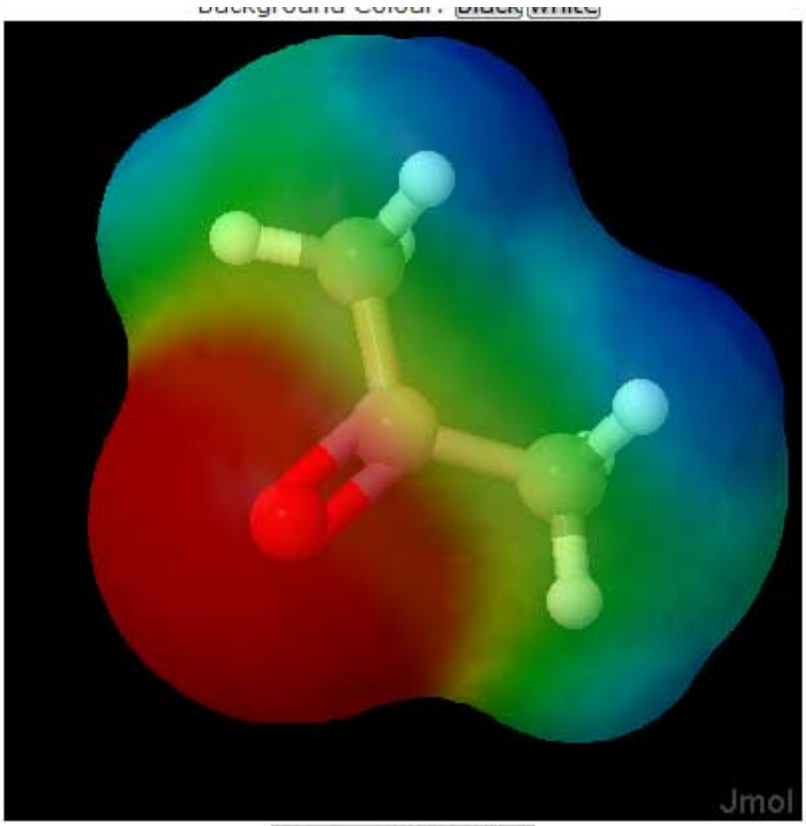
Will investigate this… may need to make decisions on features. If I had to do this from scratch…
We need to be confident we want to use these representations for dipoles. Since we are manipulating in 2d – could come up with 2d representation in 2d.(and use 3d representation on all tabs and not let users rotate).

Will it be OK in this sim to have very different representation in "Real Molecules" tab? Or will it be too much of a disconnect when you move 2d to 3d. Main concern for me.
KP: can JMOL be integrated into model of sim?
CM: hopefully it has a transparent background.
SR: if you wanted it to be 3d moveable. If you wanted to draw cube or probes you can move around are very difficult in JMOL.
CM: or to get this thing to interact with other things. I think it will work well for 3rd tab.
KL: I think that is all we really have planned.
SR: can you show other demo from JV? This is another than renders 3d surface. A little higher power 3d library.
KP: what's disadvantage.
SR: less transparent… more tweaking on our own. Also has more of a download for user because it is using native graphics libraries.
CM: if at all possible we want to avoid making modifications to 3rd party packages. Then we can't upgrade.
CM: probably will do 2d representation for first 2 tabs. May then work on 3rd tab and see 2d and 3d. Will be tricky to make 2d look like 3d.
SR: another possibility is to use 3d engine JO and I are using.
CM: one thing we talked about at polarity meeting… we have 3d need in chemistry. We don't want to end up that each sim uses different 3d library. Would be nice if it was all on one.
KP: another recommendation for JO was for you 2 to collaborate so each is doing 3d representation. "Molecule Shapes".

Here is a screenshot I took of an open source Java program showing the electrostatic surface of a molecule (attached). I just pointed the web start version of jv at 1tup-ABCEF. It's not semitransparent like in your screenshot, but maybe that could be added. The application runs atop JOGL and was very responsive. I found it mentioned in a list here.



Here's a shot of JMol doing what you need, just click "Electrostatic Surface" and "Translucent Electrostatic surface" http://www.chemtube3d.com/ElectrostaticSurfacesPolar.html. Performance was also great in this one, and nothing would prevent us from integrating JMol into our play area.



Medium (400 px)

Controls

☐Spin ☐Zoom ☐Molecular Dipole ☐Dipoles for All Bonds
☑Electrostatic Surface ☑Translucent Electrostatic Surface

07/19/11 - SMOL files

CM: Jmol feasibility testing is going OK. I've figured out how to do most of the things that we need to do, but it's slow going.

What molecules are we likely to want for the "Real Molecules" tab?
Do you know much about chem file formats? (PQF, PQR, SDF, SMOL,...)

KL: I will send you a more complete list of real molecules, but at a minimum:
H2O (water)
NH3 (ammonia)
CH4 (methane)

I used different chem file formats back in the day, but none of the ones you listed. Do you have a specific question?

CM: I'm looking for guidance on what file format(s) to use, because there are so many of them, and the documentation of the formats stinks. And the data we need (bonds, dipoles, molecular electrostatic potential, ...) is not supported by all formats. Sounds like JO/SR have used formats that worked for their specific sims without a real understanding of the tradeoffs of the various formats. And those formats are not going to work for Polarity. In fact, the only format that I've managed to make work for Polarity is SMOL, which is created using SPARTAN SOFTWARE ($1200 per license).

This application demonstrates many of the features we need for Polarity: http://www.chemtube3d.com/ElectrostaticSurfacesPolar.html

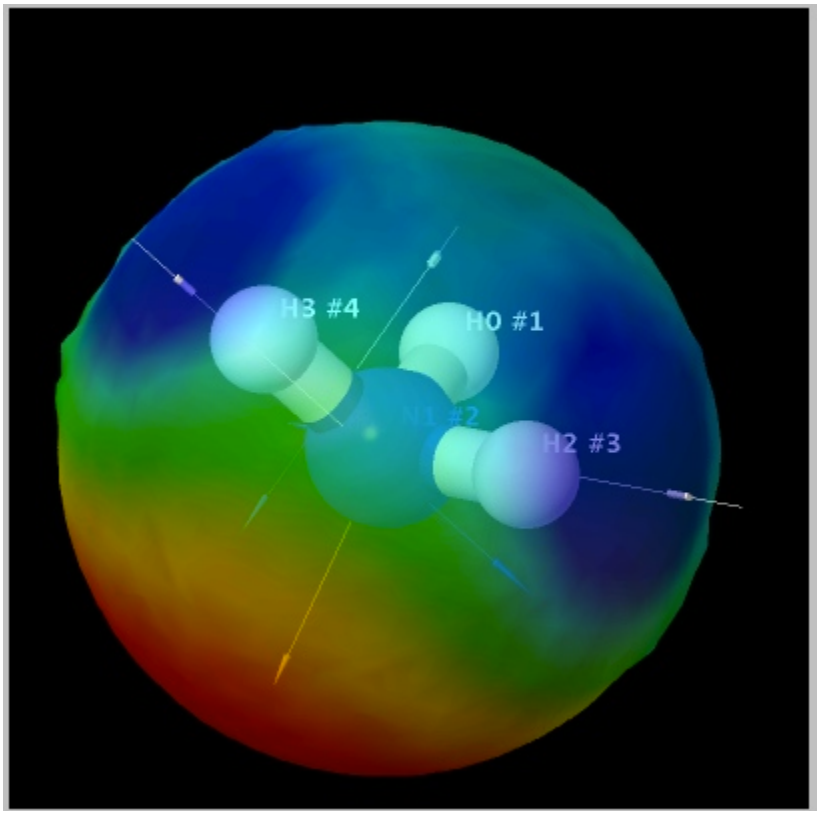
It has SMOL files for:
acetone
ammonia
boron triflouride
formaldehyde
methane
methylflouride
water

I've grabbed these files, not sure about licensing issues with reusing them.
All of them contain dipole data, and most contain molecular electrostatic potential (MEP) data.
Unfortunately, the SMOL file for water doesn't seem to contain MEP data.

KL: My old computational chemistry professor wrote code for Spartan. His group could probably do calculations on any molecule we want and give us the output (SMOL) files.

Can you send me the actual file for one of the molecules? Maybe ammonia?

CM: SMOL attached for ammonia. Also attached is a screenshot of how Jmol displays it in my test program.



KL: It looks like SMOL is the only file type that works with Jmol and includes the data we need.

Here is a page I found that shows the electrostatic potential for water:
http://faculty.trinityvalleyschool.org/pricep/jmol/molimages/water.html

I asked my old professor to do some Spartan calculations for us; I'll let you know if/when he responds.

We should only include real molecules with one central atom (so we do not need the SMOL file for acetone). Here are some options:

H2 (hydrogen)
HF (hydrogen fluoride)

H2O (water)
CO2 (carbon dioxide)
HCN (hydrogen cyanide)

NH3 (ammonia)
BF3 (boron trifluoride)
CH2O (formaldehyde)

CH4 (methane)
CH3F (fluoromethane)

07/20/11 - Versions 1&2

CM: http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.01/

I'm hesitant to show this version, because it's not very mature. But I wanted to give you a feel for how feasibility testing of Jmol is going. Please ignore everything except the "Real Molecules" tab. Any "red" controls are not implemented. The molecules in the combo box are not necessarily what we're using, they are simply molecules for which I could find data files (and they are dubious data files, in .smol format).

I started to work on the "Two Atoms" tab, and quickly discovered that I couldn't really continue with 2D implementation without knowing what 3D "look" I was trying to match. So I switched to the "Real Molecules" tab, and investigation of Jmol (features and Piccolo integration).

I've figured out how to:
- integrate a Jmol viewer into the play area (using PSwing, and there are some caveats)
- display dipoles (bonds and molecular)
- customize dipoles (offsets, widths, scaling, etc)
- display molecular electrostatic potential (MEP) (but doesn't work for "water" data file)
- turn off the right-click popup for the Jmol viewer

I have NOT figured out how to:
- display partial charge
- create a custom isosurface that corresponds to our "electron density" view (this will be a big project)
- rotate the molecule to be in alignment with the E-field
- adjust colors for the atoms (this is being done in BAM, so it's possible)
- constrain rotation to 2 dimensions (for potential use in first 2 tabs)
- adjust bond angles (for potential use in "3 Atoms" tab)
- use a transparent background for the Jmol viewer (I'm faking this by using same opaque color as the play area)

This experimentation with Jmol is slow going, because Jmol documentation stinks and I'm trying to do things that weren't done in BAM. But implementing these features without Jmol would have taken an order of magnitude longer, so it's been time well spent. I'm optimistic that I'll be able to resolve many (but not likely all) of the remaining issues.

So... The questions to ponder are:

1. If Jmol provides 90% of the needs in the "Real Molecules" tab, are you willing to jettison the 10% of features that it can't provide?

2. If Jmol is not suitable for use in the first 2 tabs, what differences in "look" between 2D and 3D are you willing to tolerate?

KP: I would vote for optimizing tabs 1 and 2 to have the features we want for attaining the learning goals and to be intuitive to use because this is where the interactivity is going to be primarily. Tab 3 is important, but I'd be pretty comfortable having some differences in the displays for tabs 1,2 versus tab 3.

<u>Status meeting notes</u>
KP: who makes Jmol? University project? Has anyone communicated with them?
JB: I think this is unusual use.
KP: would be nice if EM could communicate with PI of grant, that we are using their software in this system. They might like to know about application, might help them for grant reports.
CM: yes could help to say it is used in PhET sims…
KP: we could give them info on who uses sims.
SR: doesn't look like it is affiliated with University. Looks like passed down through people. If you google Jmol there is a link to history. Latest guy looks like he is in Minnesota.
RP: Xmol came out of supercomputer center tied to university.

What I have been doing this week is looking at 3d requirements, how to accomplish them with Jmol. SR: Jmol has built in support for electrostatic surface etc.
CM: scripting is weird, and documentation is hard to read pseudo descriptions, can be redundant or lacking information.
There is a decent amount of customization… made them a little larger diameter to make them easier to see. Offset them to make them visible (if vector were small enough).

We need to have a discussion about where we actually want them to show up. Not sure why it starts to wobble. Seems to change when I turn map on. Maybe it is supposed to be bumpy. Isosurface command that has dozens of parameters you can give to it.
KP: doesn't seem to have shape of molecule.
CM: could be matter of data files. By trial and error, found out it will work with JMOL.
NP: looks like surface map of potential.
JB: its pretty cool.
CM: for some reason, water doesn't work. No idea why.
JC: will you show boron trifluoride?
CM: might label atoms so that you can see them.

Haven't figured out how to show partial charge. Not sure if it supposed to be embedded in data file. Haven't looked around too much. Not sure how to turn field off, and figure out right rotation to get this to look like it is properly lined up with field. Can't determine orientation with respect to field.

Creating a customizable surface. We made it up. Will have to figure out how to use their isosurface

command to recolor electrostatic potential surface. Looking through it, it will probably be mini project of it's own. Colors are already done in build a molecule, so could be easy, but he is loading data in own format so then you can change colors. Complete molecule? Will probably have to do something similar or leverage what JO has already done.

Play area, background, set to same color, but if we had need to drag things behind this. Found forums where there were issues with transparency. Didn't see anything like that in requirements. Probably not general play area we can use in future projects.
SR: I don't think that it is a problem. I think there are workarounds for transparency.

Continue with partial charges, (biggest thing). I question value of electron density.
KP: would be nice to see interviews. Could be done with molecular workbench sim that is already there.
KL: other thing is electron density… probably not best word use.
CM: still ball and stick model just wrapped… probably need to revisit control panel. Maybe not even call it "ball and stick". What visualization of what charge to use.
KL: file format is proprietary software that is really expensive. I know someone that is going to generate this for us. (water, etc).
CM: only reason I ended up with Smol is there was a demo that still used these. Publically available files. (I don't know if we can even use these files).
KP: it sounds like KL knows the most
KL: we can get someone to generate files, and as long as we cite them, we should be alright.
CM: there is a big block of stuff, binary data that is converted to [sd]?
AP: person you know that did coding might have idea
KL: there is calculation you are running, and output file he is using. I see what file is saying, but don't know what is happening – don't know how they are taking that info and creating surface in Jmol.
CM: PDB is file type in BaM and SaSS. BaM started with pub chem SDF.

Got some to work with PDB some to work with SDF.
JO: I know sdf's have a lot of info, but they are different 2d and 3d files, contain different information about the molecules, had to combine the 2 and pull info I needed from both. They have a lot of information on each.
CM: was going to try to get SNF file, convert to PDB, then a server to convert to PQR.
KP: can we continue this offline?
CM: spending a lot of time thrashing on file formats.
KL: only documentation was using SMOL file from Spartan.
JO: I have had some experience digging through that kind of stuff.
CM: is this looking how you want to look? Or will these never work?
KL: could make them smaller and thicker.

Team meeting notes

- TL: should we show 3D vector addition?
- EM: do students think about vectors or bonds?

- put vectors *along* bonds
- KP: can we make the molecule transparent? EM: or atoms smaller?
- test offset in interviews

CM: http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.02/

This version adds Developer controls to facilitate experimentation with Jmol:

• "Import from file" - This option was added to the Molecule comb box in "Real Molecules" tab. Selecting this option will open a file chooser, where you should select a molecule data file. Since this feature requires secure access to your file system, you'll need to download the sim JAR.

• "Jmol Script" text area - Appears below the Reset All button, you can enter Jmol scripts here. Press the "Run Jmol Script" button to execute the script. Jmol's scripting language is documented at http://chemapps.stolaf.edu/jmol/docs

For both of these features, you should have your Java Console enabled, since Jmol writes diagnostics to the Console.

07/21/11 - Jmol contact

CM: (to Emily) In yesterday's status meeting, Kathy asked you to make contact with someone at Jmol, to inform them of how PhET is using their product. When you do that, could you please also ask them what are the most effective ways of getting technical support? I don't plan to bug them right away, but it would be good to have a technical contact for future issues.

KL: This guy has shown up in a bunch of online Jmol discussions:

Robert Hanson
Professor of Chemistry
St. Olaf College
Northfield, MN
http://www.stolaf.edu/people/hansonr

CM: Discussions where?

KL: http://sourceforge.net/mailarchive/forum.php?forum_name=jmol-users

Here are all the entries about smol:
http://www.mail-archive.com/search?l=jmol-users%40lists.sourceforge.net&q=smol

KL: Can you send me the smol files for HF and BF3? They are the only ones that do not have a spherical electrostatic potential map.

Also, has anyone contacted Bob Hanson <hansonr@stolaf.edu>?

CM: Requested files attached. They are also in SVN under trunk/simulations-java/simulations/molecule-polarity/data/molecule-polarity/jmol/.

I have not contacted Bob Hanson. I wasn't planning to until Emily has established a Jmol contact, and until we have a clear idea of what we want to contact him about. I also feel that posting to the forum is preferable to contacting people directly, because it benefits others who many be experiencing the same issues, and allows contributors to respond when they have time.

07/21/11 - Help with Spartan

KL: I hope all is well in Atlanta!

I work for a project that develops free online simulations to help students learn science: http://phet.colorado.edu

We are working on a new sim about molecule polarity, and we want to use Jmol to show bond dipoles in 3D. Jmol reads the .smol output file from Spartan calculations, but we do not have access to the software.

Could you do a quick geometry optimization (at the B3LYP/6-31G* level) for a handful of small molecules? We also want to show electrostatic potential maps, so we'd need you to compute Surface info. We do not need vibrational modes, etc.

We'd cite you and Spartan in the credits.

DS: I'm in Spain right now, but perhaps my student Trent Parker, or one of my other students, might be able to assist. I'll copy Trent on this.

TP: I could definitely help out with this. I would just need to know which molecules you wanted and which conformer if there are multiple conformers.

KL: The molecules we need are very simple:

H2 (hydrogen)
N2 (nitrogen)
O2 (oxygen)
F2 (fluorine)
HF (hydrogen fluoride)
CO (carbon monoxide)

H2O (water)
CO2 (carbon dioxide)

HCN (hydrogen cyanide)
O3 (ozone)

NH3 (ammonia)
BH3 (borane)
BF3 (boron trifluoride)
CH2O (formaldehyde)

CH4 (methane)
CH3F (fluoromethane)
CH2F2 (difluoromethane)
CHF3 (trifluoromethane)
CF4 (tetrafluoromethane)

I included more than we may use, because I don't want to bother you again :)

Many are probably already in the Spartan database, so you may only need to do energy calculations to generate the SMOL files.

Here is a link to a crude version of the sim:
http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.01/
(Click on the "production" link)

You can skip to the "Real Molecules" tab to get an idea of how we plan to use the Spartan data.

TP: The geometries, surfaces, etc. are all quite easy and quick to do. Regarding the output, is the output format you want the standard Spartan output file? (i.e. from the Display -> Output (Verbose Output) menu?) Or is some special output type necessary? Our installed version of Jmol does not read this .spartan output. The program does not give any other option for file type to save besides the .spartan extension.

Also, do you need a specific isodensity value for the ESP output? The program's default value is 0.002.

I have attached the output file for O2 for you to see if it meets your request.

KL: Thank you for the output file, but the spartan format did not work on our end either.

It could be that smol is an old file type that is no longer supported in Spartan. Can you try to export the O2 file in a different format? sdf, mol, etc.

The default value for the isodensity is probably fine.

TP: Attached are several forms of the saved Spartan output. I was unsuccessful again in finding

the .smol format.

The .mol file is rendered as dummy atoms.
The .mol2 file does not read.
The .txt file does not render. This is the abbreviated Spartan output file.
The .sdf file will render a molecule, but this file only contains the geometry, not ESP information.
The .spartan file will not render, but contains all of the detailed information about the molecule.

The .spartan file contains the detailed information about the basis set exponents and wavefunction (Hartree-Fock C Matrix) from which the ESP could be reproduced. This seems to be the crucial file.

Do you have a sample .smol output file I could see? I could see if any file formats resemble it or could be altered to its format.

KL: Thank you for sending the different types of files. Here is a sample .smol file for ammonia. I appreciate your help!

KL: I figured out a way to make mol2 files work for our needs in Jmol. Could you send me the output files for all the molecules in mol2 format?

I want to thank you for all of your help! I will let you know when we post the final version of the sim on our website, but for now, here is a link to the latest version:
http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.03/

And can you add one molecule to the list: CHCl3 (chloroform)?

TP: All the .mol2 files are attached (including chcl3)

KL: Thank you for the mol2 files!

The first mol2 file you sent for CH2O had partial charge info, but the new mol2 files do not. Did you use a different command when you exported the files? We need the charges to generate the dipoles and electrostatic potential.

TP: Spartan gives three options for saving charges: Electrostatic, Mulliken, or Natural. I assume that you want Electrostatic. Is this correct?
KL: Yes

TL: Updated files with electrostatic charges are attached.

KL: We integrated the mol2 files in this version:
http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.05/

07/21/11 - Jmol file formats

CM: Since identifying a suitable Jmol file format has become a mini project, I've created ticket #3018 to keep track of resources, our experiments, etc. If anyone has anything to add, feel free to do so.

KL: Can you try these out? I asked Trent to export the spartan file as other file types. I doubt any of them work.

CM: Au contraire. See test results in comment 9 of #3018. This is somewhat baffling to me...
KL: The ch2o-sdf.jpg looks like ammonia.

CM: Ah, yes indeed, my mistake. Looks like I forgot to change the combo box selection for that one. Ticket updated with proper sdf results (doesn't display dipoles or mep). I was surprised that mol2 display everything.

KL: Jmol must be calculating the dipole and electrostatic potential from the atomic charges in the mol2 file. But the file contains no electron density information, which may be why the surface is just a sphere.

KL: I figured out how to generate the electrostatic potential map from the partial charge data. The water file works now.

Run the Jmol script: isosurface VDW map MEP colorscheme "RWB" translucent
in the dev version:
http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.02/

CM: I switched to your list in http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.03/,
and I'm loading SDF files obtained from PubChem (see SDF button at upper right).
I'm also using the "isosurface" command that you specified.

3 of the molecules don't display MEP - boron trifluoride, hydrogen, methane.
As requested, I'm attaching all of the SDF files.
The 3 files prefixed with "X" don't display MEP, they are missing partial charge.
"X-2D" are 2D files, "X-3D" are 3D.

Btw... The mol2 files are easier (for me) to understand and modify. For example, I don't see an obvious way to change the atom labels in the sdf files.

KL: In the sim, can you list the molecules in the order I sent? They are in order of size/complexity. I asked Trent to make mol2 files for us.

CM: http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.04/

I figured out how to do some more things in Jmol. Below is a list of changes, all in the "Real

Molecules" tab. Some of this is for purposes of demonstrating Jmol capabilities, and much tweaking of colors, positions, etc. needs to be done.

Changes:
- order molecules in combo box by increasing size/complexity
- increase font size (18pt) for all atom labels
- set color=black for all atoms labels
- display partial charge as part of atom label (haven't figured out how to display it separately)
- demo of bond customization: make bonds black and slightly thinner
- demo of transparency: make bonds and atoms translucent when dipoles are visible
- demo of custom atom colors: use custom colorblind-red for oxygen atoms
- disable hovers, so that labels don't become visible when you put the mouse over an atom)
- disable shift-drag zooming

Also note that the default selecting in the Molecule combo box is H2, which is one of the broken SDF files.

07/28/11 - mol2 files

KL: Here are the mol2 files. I asked Trent for more molecules than we may use.

CM: Do you want me to make all of these accessible from the Molecules combo box (for now)?
KL: Will it fit on the screen?
CM: They will just fit, and I can make the font a tad smaller if necessary.
KL: Ok, let's add them all for now, and then we can decide which ones to keep later.

See https://phet.unfuddle.com/projects/9404/tickets/by_number/3025

CM: OK, will do. Can you please note the names that you want to use next to each of the file names below? And please indicate the order you'd like them to appear in the combo box.

H2 (hydrogen)
N2 (nitrogen)
O2 (oxygen)
F2 (fluorine)
HF (hydrogen fluoride)
CO (carbon monoxide)

H2O (water)
CO2 (carbon dioxide)
HCN (hydrogen cyanide)
O3 (ozone)

NH3 (ammonia)

BH3 (borane)
BF3 (boron trifluoride)
CH2O (formaldehyde)

CH4 (methane)
CH3F (fluoromethane)
CH2F2 (difluoromethane)
CHF3 (trifluoromethane)
CF4 (tetrafluoromethane)
CHCl3 (chloroform)

CM: All of these files are missing partial charges, and therefore cannot render MEP.
KL: Ugh. Can you send me the new mol2 file for CH2O? That was the one that worked before.
CM: Latest ch2o.mol2 attached.

CM: I integrated these mol2 files into this dev version:
http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.05/

Jmol reports that H2, N2, O2, F2 are all missing partial charges. Looks like maybe the partial charge values are zero in the files?...

Here's the Java Console output:
> eval ERROR: No partial charges were read from the file; Jmol needs these to render the MEP data.

The other molecules look OK (to me, but you should check them.)

KL: I think the molecules look great! At some point, I'd like to tweak the axes so you can see all of the atoms in the molecule when it comes up on the screen.

I had not thought about it, but yes, H2, N2, etc. do not have partial charges. We could:
- disable the electrostatic potential for those molecules
- use the VDW surface and color it transparent white: isosurface VDW color white translucent
- not use those molecules: I had only planned to use one of them anyway

We can decide which real molecules to keep in the sim at the next Polarity meeting. I think having them all in the combo box for now will help us decide.

CM: Agreed. I think I'm also going to need to know how the initial orientation relates to the orientation required for E-field alignment. It would be ideal if this were the same for all molecules. Otherwise we'll need to either (a) investigate whether we can put a property in the mol2 files that describes this, or (b) hardcode for specific molecules.

Is there a general rule for determining when a molecule will not have partial charges? Something like "if the molecule is composed of homogeneous atoms, it has no partial

charges"?...
Just trying to figure out how I can tell when to do something different (disable MEP, use VDW,...) without hardcoding for specific molecules.

KL: The general rule is:
Molecules composed of *two identical atoms* do not have partial charges.
CM: So ozone (O3) does have partial charges?
KL: Yep

08/03/11 - Versions 6&7

CM: http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.06/

"Two Atoms" notes:
- added partial charges view
- added bond type indicator
- molecule rotates to align with E-field (angular velocity is proportional to dipole magnitude, no angular acceleration)
- all scaling factors (for animation speed, fonts, vector lengths, etc.) are easy for me to change
- "Electrostatic Potential" and "Electron Density" features are not implemented (waiting to see what we do in Real Molecules tab)
- I plan to improve some of the graphics in this tab (add cross to dipole, add perspective to E-field plates, snazzier bond type indicator,...)

"Real Molecules" notes:
- switched to mol2 file format, added many more molecules (will likely drop some)
- molecules are ordered in the combo box by increasing complexity
- molecules with 2 of the same atom (eg, H2) have no partial charges. How do we want to handle this? Drop them? Disable features?
- partial charge is currently displayed in the only location supported by Jmol: with atom labels. Is this acceptable?
- if we want to label atoms differently, we'll need to manually edit the mol2 files
- if we want different initial orientation of molecules, we'll need to either manually edit the mol2 files, or build a table of initial rotation values
- turning on dipoles currently makes the atoms and bonds translucent, to show you what this looks like, for discussion purposes
- dipoles are displayed using Jmol's default scaling and offsets
- E-field alignment is not implemented, I need to look into out how to get the molecular dipole angle from Jmol
- "Electron Density" view is not implemented
- Jmol sometimes fails to render atoms until you start rotating the molecule

KL: The first tab is looking good! I like the molecule rotation, but I wonder if we should make it so that the molecule is in a position to rotate if the student turns on the electric field before doing

anything else. I can see what students do first in interviews.
CM: Trivial to change, just let me know what initial rotation angle you'd like. Rotation angle is currently 0, and positive rotation is clockwise.

In the real molecules tab:
- the atom labels should be on by default
CM: Trivial, done.

- if there is only one of an atom in a molecule (e.g. HF), the atoms should be labeled H and F (i.e. no numbers); if there are 2 or more of an atom (e.g. H2), the numbers should start at 1 (i.e. not 0)
CM: After much experimentation, my conclusion is that Jmol does not support this format. If you want to experiment further using the "Jmol script" box, see the label command and the various atom properties. With both labels and partial charges enabled, I'm currently using this Jmol script:

label %[element]%[atomIndex]|\u03b4=%.2[partialCharge]

Jmol seems to be lacking an "elementIndex" atom property.
If we can't resolve this, we'll need to manually edit the atom names in the mol2 files.

- it would be nice if the partial charges did not push the atom labels off the atoms; can the charges go on a separate line?
CM: Done, see above "label" command, where '|' is the line separator.

- the electrostatic potential feels like it should be a checkbox
CM: The entire "Model" control panel should be rethought, so I'm not going to change this now.

If "electrostatic potential" is the only isosurface view, then yes, it can be moved to the View control panel and converted to a checkbox. If we have multiple isosurfaces, then "Model" should be renamed, and the choices should be "electrostatic potential", "electron density", and "none" (or whatever the user-friendly labels are for these choices.) That said...

Creating the "electron density" view is going to (at the very least) double the amount of time we spend on isosurfaces. And since it's a nonstandard representation that PhET has made up (and has yet to adequately specify) I question the value of this feature relative to its cost. It would be nice if a decision could be made on this in the next week. Is the "electron density" in or out? If it's in, specify it fully (colors, shape, etc.) and figure out how to do it with Jmol. Once this decision is made, I can get to work on changing the control panel, and implementing the 2D versions of Jmol isosurfaces.

- for molecules with 2 of the same atom, can you try the script I sent you for the electrostatic potential?
CM: I can't give you a dev version that uses your script (see below). But you can enter your

script in the "Jmol script" box to confirm that it works, and it does appear to work. The script is "isosurface VDW color white translucent".

In order to use different scripts for different types of molecules, I need to interrogate Jmol about the molecule. Extracting information about the molecule from Jmol is nontrivial, so I'll need to work on this. It involves writing a Jmol script that iterates over the atoms, counts element types, determines if we have a "2 of the same atom" molecule, then passes this info back to Java.

KL: We can work on editing the mol2 files when you return from vacation.

JC: I like the first tab a lot; playing with the electric field is fun!

My only comment is that many of the linear molecules I tried in the "real molecules" tab appear with the viewer looking down the line of the bond, so that it looks like a single sphere. The viewer has to turn the molecule 90 degrees so that it is in the plane of the computer screen, in order to see it better. Can this be changed so that linear and diatomic molecules appear in an orientation that looks like the 2 atom tab, with the line of the bond in the plane of the computer screen (not pointing toward the viewer)?

CM: Jmol provides no ability to programmatically determine what is and is not visible in the initial orientation, so I cannot adjust the initial orientation to ensure that all atoms are visible. The orientation displayed is the orientation that was used when the mol2 files were created. I have no idea what was used to create the mol2 files, or whether initial orientation can be changed at that stage. (Perhaps Kelly can elaborate).

Our choices for solving this problem are (in order of decreasing desirability):
(1) create the mol2 files with the desired orientation
(2) manually edit the mol2 files to give the desired orientation (becomes more difficult as molecule complexity increases)
(3) create a table of rotation angles to be applied for each molecule (will make the implementation fragile and harder to maintain)

EM: First tab is looking great! Can't wait to be able to play with changing the electrostatic potential.

KL: Is a different colorscheme all we really need for the "electron density" isosurface?

Run the script below in the dev version:
isosurface VDW map MEP colorscheme "BW" translucent

Kathy: is this close to what you want?

CM: I've implemented this "electron density" representation in:
http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.07/

Note that the "Model" control panel is now labeled "Isosurface", and it has 3 choices.
These are obviously not the labels we want to use for the end product, but it's something to start with for discussion purposes.

KL: (to Julia) we are planning to rotate the initial positions of the real molecules by editing the xyz values in the mol2 files. For example:

	x	y	z
A	0	0	-1
B	0	0	1

would be:

	x	y	z
A	-1	0	0
B	1	0	0

The molecules are oriented to exploit as much symmetry as possible, so it should not be too hard to change the major axis.

CM: Before we put too much time into tweaking the mol2 files... I'm not clear on whether we've made a decision on file format. Are we going to stick with mol2 file format? Should I close #3018?

Are you sure about this for all molecules? Some would be nontrivial to edit by hand. For example, here are the xyz values for CH2F2:

C1	0.000000000	0.000000000	0.508880522
F2	-1.109124829	0.000000000	-0.279924737
F3	1.109124829	0.000000000	-0.279924737
H4	0.000000000	-0.909431633	1.120073924
H5	0.000000000	0.909431633	1.120073924

That's not something that I'm excited about manually editing, and definitely not more than once. If we have even 1 or 2 like this, then it would be far better to specify the initial orientation when the mol2 files are created, rather than editing them by hand. Is that possible?

TL: I wanted to see how things are progressing because I noticed that the surface color was up for discussion and I was curious about how the vector representation was progressing. I'll be teaching regular HS chemistry and I see that being able to determine polarity is part of our district chem program, not just the honors program. That means many of my students will not have any experience with vectors since vector math has been removed from math curriculum that is typically the pre-requisite. I think they may understand the electron density mapping (like

the surface map) better because they have extensive experience with contour maps. I didn't like the red-blue colors because I was fairly sure it would be confusing for my students. Red usually denotes positive and they get confused when red is used for "less-negative". So here's my thoughts:

I think the "isosurface VDW map MEP colorscheme "BW" translucent" looks good on my flat-screen and on my laptop. I'll be back at school on the 17th if you want input about projection, but I could go to school earlier if it would be helpful.

I really like the way the Molecule Dipole vector looks because it radiates out from the central atom and is very distinct because of the transparency of the atoms and bonds.

Another improvement that I have noticed is that the vectors are only one color now; when the vectors were two-toned , I thought it would be confusing much like the red denoting "less negative".

I am not necessarily saying that mol2 format is positive or negative, I am just giving my input on my thoughts about the improvements on color schemes, transparency, and how the molecular view changes to allow the molecular dipole and electron dispersion to be more predominant.

KL: Two Atoms:
- "bond dipoles" should be singular in this tab

Real Molecules:
- let's stick with the mol2 format
- The linear molecules are the ones that start with the atoms going into the screen, and they are trivial to change. The ones that could pose a problem are:
CH2O
CH3F
CHF3
CHCl3
You can change the initial orientation of the molecule in Spartan, but many programs try to align the molecule to use symmetry in the calculations. I can ask Trent to turn the symmetry off, but first let's try to edit the files.
- we can easily change red to "positive" and blue to "negative" by using the "BWR" colorscheme instead of "RWB"

CM: I'll start working on initial orientation of the mol2 files. If there are any complicated (not linear) molecules that you want changed, please send a screenshot showing the desired orientation. I'll also edit the atom names in the mol2 files, so that they are indexed by atom type (eg, CH2O -> C1,H1,H2,O1)

Do you want me to change MEP colorscheme to RWB? Or were you just proposing this as a solution to Trish's concern? Is there a standard convention for this? For example, if textbooks

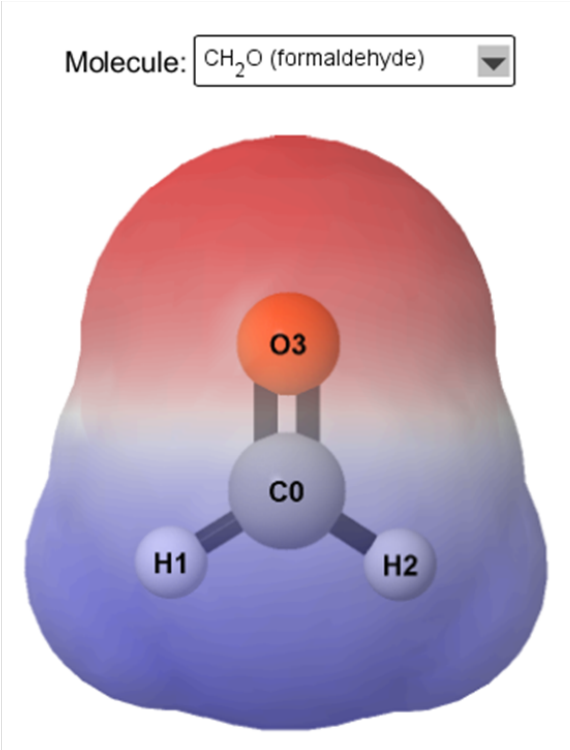
use BRW, then I would certainly be concerned about using the opposite.

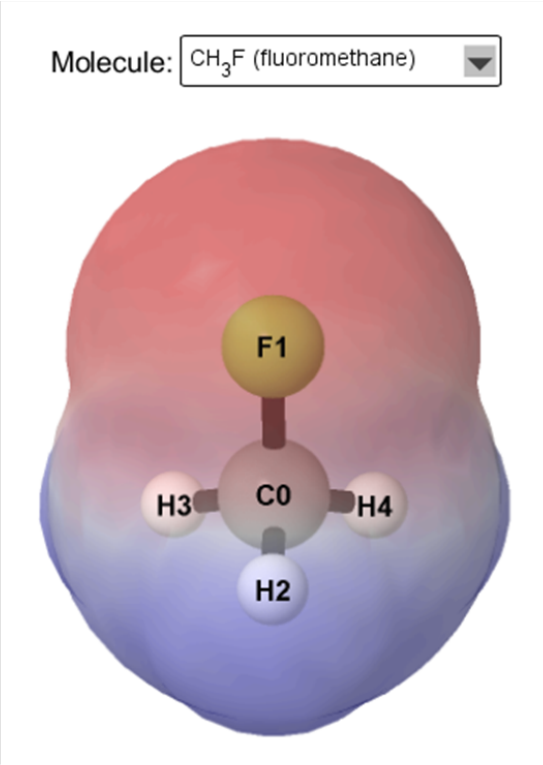
KL: Great! For the linear molecules, change the axis from z to x.

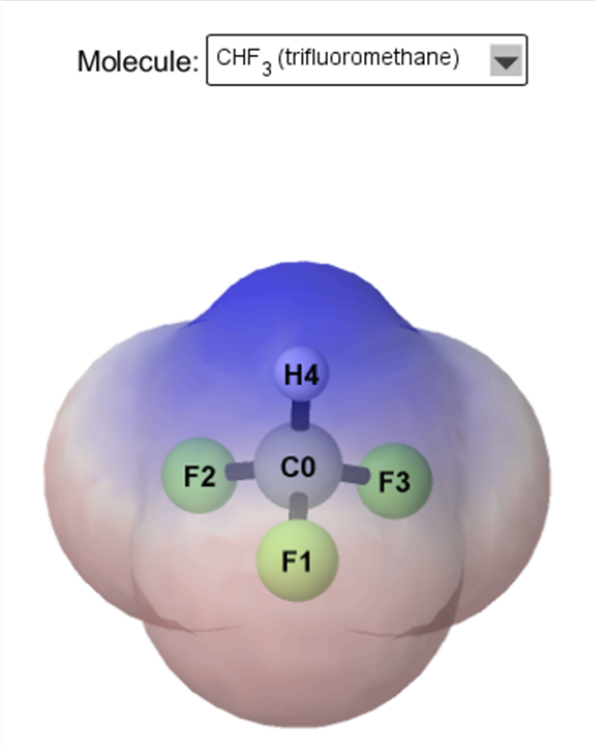
HF: put H on the left, F on the right
CO: put C on the left, O on the right
HCN: put H on the left, N on the right

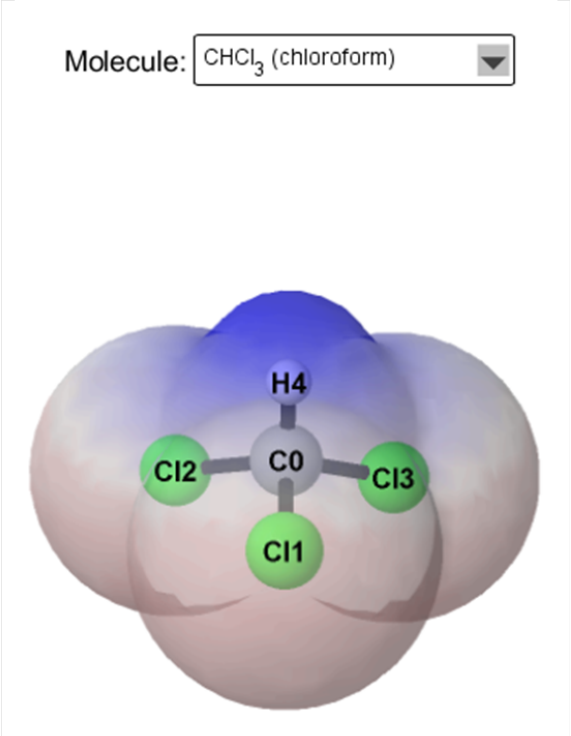
I attached screenshots for the non-linear molecules.

I was only saying the colorscheme is easy to change and test in interviews. The convention is how we have it now: RWB, or red for low potential, blue for high potential. But I'd like to see if this is confusing for students before we try the opposite.







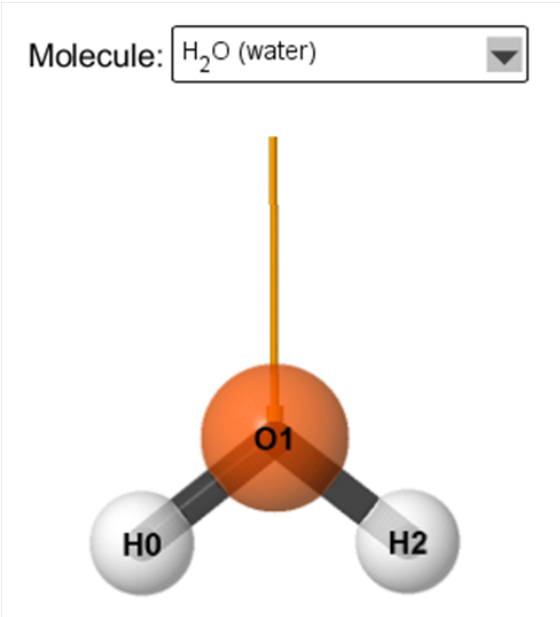


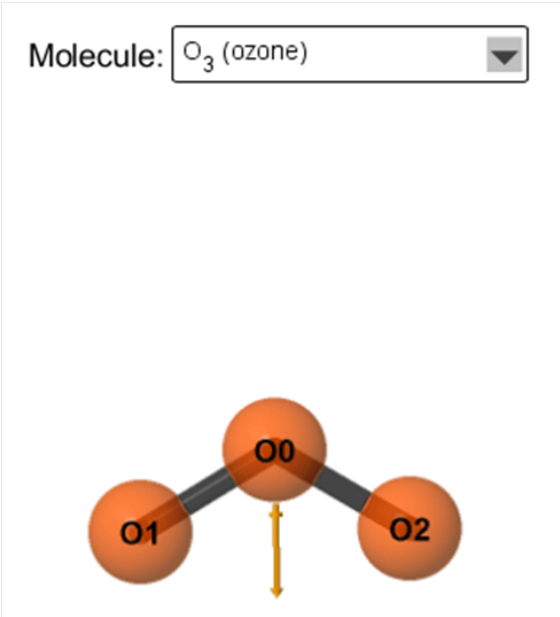
CM: Did you consider the orientation of the molecular dipoles in choosing default orientations? For example, H2O's molecular dipole currently points straight into the screen, the student will never see it unless they rotate the molecule.

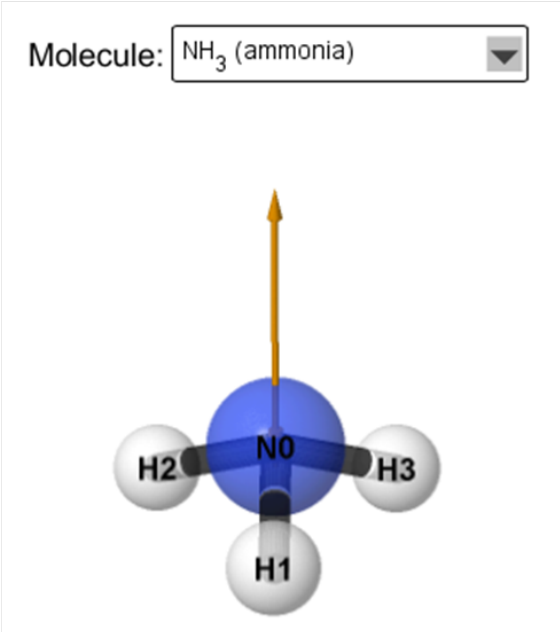
KL: No, for this first pass I only wanted all the atoms in the molecule to be visible.

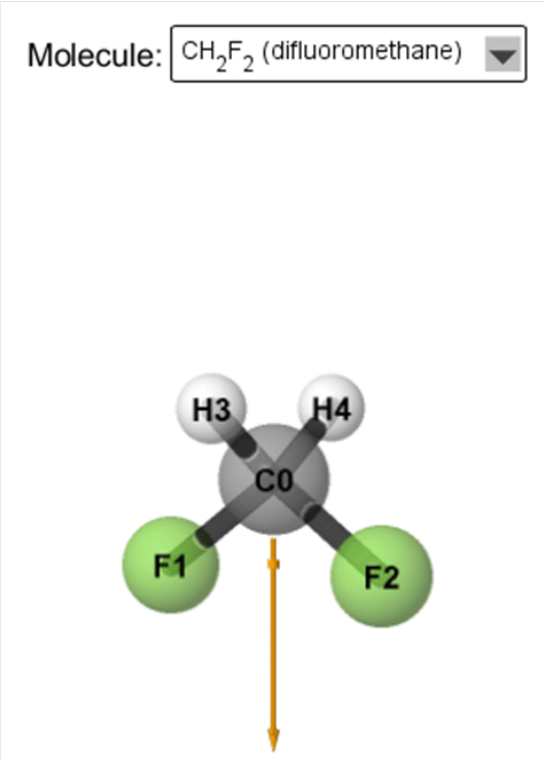
The molecular dipole is hidden for:
H_2O
O_3
NH_3
CH_2F_2
assuming we rotate the other molecules as specified earlier.

Here are options for those 4 molecules.









CM: Do you want me to implement these, or do you want a "first pass" in their original orientation?

For changes that don't involve a simple axis swap/inversion (rotation about 1 axis), I will need to write code to transform the xyz coordinates.
Based on your screenshots, that includes these molecules:
CH3F

CHF3
CHCl
NH3
CH2F2

KL: Yes, implement all the new orientations. Thanks!

08/10/11 - Meeting day

Bond type indicator
- get rid of line arrows & word “more”
- add a label
Dipole vectors
- make look like Jmol vectors
3-atom tab
- how to rotate molecule & change bond angle
- where to put dipole vectors

<u>Notes from status meeting</u>
CM: Most of 1st tab done. Everything not done – things we need to make a decision about. What do we want iso-surfaces to look like? So, I propose we put a deadline on when we are going to decide how we want these to look. Do we want red/blue. Want them to be flipped? Can’t do anything over in 2d until we come to conclusions on 3d. Pick a time?
KP: this one looks good to me. Unfortunate that it is such an issue with how PhET is oriented now.
CM: I think we should decide how we should decide. Can delegate decision?
KP: I would like to hear the discussions.
CM: rainbow still on the table. Used in textbooks and common representation.
KP: it is pretty easy to delete electron density view. I will play around with it.
CM: That is big impedance for getting to interviews and seeing if other things are working well.

CM: Bond type thing – simple continuum. It goes to extreme of continuum. Or do we want arrow to stop before it gets to end? Should it be labeled “bond type”?
TL: I know I had to figure it out. But I had context.
KP: a label seems useful.
JC: could use nature of bond and could put “more covalent” etc.
KL: we had in previous version but arrow is telling you it is more of this or more of that.

CM: Bond and molecular dipole vectors – need to come to consensus on that too. Doing whatever Jmol defaults to currently. So we still need to decide on that. Making things transparent now. When dipoles are on.
Really need to start nailing it down so I can finish this puppy up.
If we want to put dipoles inside the bonds the transparency could be an issue.

CM: A few other things about manually going in and changing labels on Atoms. Jmol indexes atoms in order it gets them.
Partial charges are still a little noisy. If you turn off atom labels it becomes easier.
MD: could you have them float just outside?
CM: yes can offset, but when I have them offset they won't be centered.
Can also control whether they float on top of everything – or could make it go behind.

08/12/11 - Polarity questions

CM: Is this what we decided for molecules like "H2" in the "Real Molecules" tab?

- uncheck and gray out "Bond Dipoles" and "Molecular Dipoles" check boxes
- use "isosurface VDW color white translucent" for "Electrostatic Potential" isosurface

And what should I do for "Electron Density"?... Nothing for now?

Is there a more specific name for "molecules that are composed of 2 of the same atom" ?

KL: One of the learning goals is that "homogeneous diatomic" molecules do not have a bond (or molecular) dipole, so we should not disable the dipole checkboxes. For now, use the same script for the "electrostatic potential" and "electron density" isosurfaces for those molecules.

CM: How will students distinguish between no molecular dipole and a zero-length molecular dipole?

KL: Are those not the same thing? In the Two Atoms tab, you do not see a bond dipole when the atoms are the same (same EN value); the Real Molecules tab should be consistent.

CM: In general, a zero-magnitude vector is different than "no vector". But it sounds like "zero-length dipole" and "no dipole" are synonymous in this domain. Is that correct?

KL: I guess you can get a zero-length molecular dipole if non-zero bond dipoles add to zero.

CM: In the "Real Molecules" tab, partial charges are quantitative, displayed as (for example) "d=0.42". Does this display require units, or should it be something like "d=0.42e"?

KL: Hmm. This may be a good question for the team. For now, leave the units off. Also, we could show d=0.42 as d=+0.42. What do you think?

CM: Not sure if Jmol gives me any control over that, but I'll check.

08/12/11 - Version 8

CM: http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.08/

Lots of changes in this version, as detailed in the changelog at the above link. Big stuff that's still in the works:

Two Atoms:
- refine the isosurface shapes and apply color scheme
- add snap-to-ticks for electronegativity sliders

Three Atoms:
- all of it

Real Molecules:
- change initial orientation for NH3, CH3F, CHF3, CH2F2, CHCl3
- figure out how to align molecular dipole with E-field (no idea how I'm going to do this, since Jmol can't tell me the molecular dipole orientation)

Here's a list of pending design decisions:
- color scheme for "electrostatic potential" isosurface
- requirements for "electron density" isosurface (color scheme, shape, differences for homogeneous diatomic molecules,...)
- location of bond dipoles relative to bonds
- location of molecular dipoles relative to molecules
- location of atom labels and partial charges in "Real Molecules" tab (offset or centered? always in front, or allow occlusion?)
- units for partial charge values in "Real Molecules" tab
- labels for isosurface controls
- should the pointer move across the full range of the Bond Type indicator?
- decide on final set of real molecules

EM: I really enjoy playing around with the first tab…turning the electric field on and off and watching the arrows change is a lot of fun. I can't wait until the electrostatic potential mapping is functional!

Here are a few minor thoughts I had while playing with Molecule Polarity:

First Tab:

- Changing electronegativity doesn't do anything until bond dipole or something is checked 'on'. Perhaps the sim should start with bond dipole selected 'on'. (I know this type of thing isn't important right now, but just a thought).
- Bond dipole changes length for large electronegativity difference, but seems to change size only for small electronegativity differences. This looks a little odd to me, but it's minor. You might want to check out gravity and orbits to see how those arrows scale, to see if you like that way. It's essentially the same, but the size change is more continuous down to smaller arrow sizes.

Third Tab:

- The color contrast between the highlighted 'white' and the other colors on the periodic table aren't different enough to attract much attention. Perhaps there can be a larger contrast, like deep grey for 'unhighlighted' and white for 'highlighted'. These are just suggestions, I don't care what colors they are, I'm just suggesting that a greater contrast might be helpful.

Kelly: Molecule Shapes may be ready soon for a few initial interviews. We should discuss the timing of this, so maybe we can show both sims for some preliminary feedback.

CM: I don't see a different here, can you elaborate? Both Molecule Polarity and Gravity and Orbits are using the same phetcommon code for vectors. The rule for scaling is that when the arrow length is less than 2x the length of the arrow's head, the entire vector (head and tail) begins to scale. This behavior looks the same to me in both sims. Molecule Polarity adds a cross to the arrow, and the cross scales continuously (to be consistent with Jmol, as requested).

EM: I think the difference is that in Gravity and Orbits, the range of arrow lengths is different than in Molecule Polarity. The arrows tend to be longer most of the time in Gravity and Orbits, so the change from getting shorter in length to entire arrow shrinking is less noticeable.

In Molecule Polarity, when you have only 'bond dipole' selected the only thing that changes is the arrow size so it's very noticeable that it changes from getting shorter to shrinking. Since it's so noticeable, perhaps students might attribute some meaning to that change, or be distracted by it.

CM: Ah, I see. I'm not sure how we can practically address this in Molecule Polarity. The maximum length of the dipole is currently the same as the distance between the centers of the atoms. And the length of the dipole varies linearly with the difference in electronegativity between the 2 atoms. So if we want to address this distraction, we'll need to increase the maximum dipole length (which will cause problems when rotating the molecule) and/or use a nonlinear relationship for dipole length (which is liable to cause misconceptions.)

Btw... Jmol's behavior is to scale the entire arrow (head and tail) all of the time, and we're trying to match Jmol's behavior where possible. Would doing that alleviate or exacerbate the problem?

EM: I don't think it would exacerbate the problem to have a consistent scaling method across the entire range…but I haven't been involved with any other discussions about the arrow so perhaps there are specific reasons for its current behavior.

CM: The current behavior is based on project-wide consensus. Several years ago we had a meeting about how arrows (vectors) should scale, trying to solve the problem of what to do when the arrow length is less than the arrow's head size. The goal was to have consistent behavior across all PhET sims. The behavior you see in Molecule Polarity is what we decided on, and it's implemented in the PhET common library. Some older sims may exhibit different behavior, but all newer sims should be using this library. If we choose a different behavior for dipoles, we'll be deviating from the PhET standard. And since the distraction you've described

is a general issue, we may need to revisit the issue for all sims.

KL: I like the new E-field plates and the new orientations of the real molecules!

- I agree that "bond dipole" should be on by default in the 2-atom tab.
- The purpose of the periodic table is not clear to me. What do we want students to do with it? We only use H, B, C, N, O, F, and Cl in the sim. Do we really need to show all the elements? Maybe it should be an electronegativity readout instead. At the very least, the PT should be minimized on startup.
- I can't get Molecule Shapes to run on my computer :(

CM: I'll put a "View" check box for the Periodic Table on the "to do" list.
But I'll defer working on that until the team has decided on whether this feature has a purpose.
(And I agree that this feature doesn't seem to be very useful.)

08/16/11 - Version 9

CM: http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.09/

This version is for discussion at tomorrow's Chem meeting. Please review this version and the list of design issues (below) before the meeting. It's unlikely that we'll have time to discuss all of the design issues, so I have listed them in the order that is most important to keeping implementation moving forward.

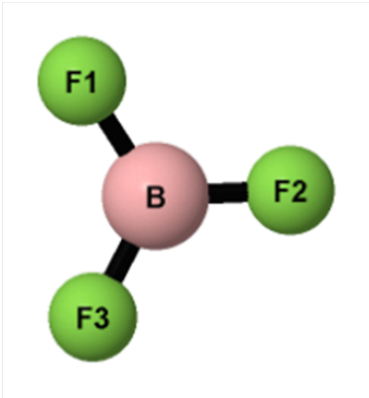
Not implemented:
Two Atoms:
- shape and color scheme for isosurfaces
Three Atoms:
- molecular dipoles
- variable bond angles
- partial charge for atom B
- alignment of molecular dipole with E-field
- shape and color scheme for isosurfaces
Real Molecules:
- alignment of molecular dipole with E-field

Design issues:
- requirements for "electron density" isosurface (color scheme, shape, homogeneous diatomic molecules,...)
- color scheme for "electrostatic potential" isosurface
- what is the purpose of the periodic table, why do we have it?
- how should the dipoles scale?
- what to show for triatomic molecule partial charges
- location of bond dipoles relative to bonds

- location of molecular dipoles relative to molecules
- location of atom labels and partial charges in "Real Molecules" tab (offset or centered? always in front, or allow occlusion?)
- should the pointer move across the full range of the Bond Type indicator?
- units for partial charge values in "Real Molecules" tab
- labels for isosurface controls

KL: Thank you for sending out the discussion questions!

In place of the periodic table, what do people think about the attached image? Or we could put the electronegativity values *on* the atoms in the molecule.



H	B	C	N	O	F	Cl
2.1	2.0	2.5	3.0	3.5	4.0	3.0

EM: I think we need to be clear on what the goal is. I believe (though I could be wrong) that Kathy's original idea for the periodic table was that students would begin to correlate the location of atoms in the periodic table with the type of bond they form. (more ionic bonds tend to be formed by elements from opposite sides of the periodic table, while more covalent bonds tend to be formed by atoms on the same side of the periodic table).

Your new representation seems to be emphasizing the differences in electronegativities. I like this new representation. It seems more consistent with the learning goals of the sim (connecting the ideas of polarity, electronegativity and geometry).

CM: The information in the table makes a lot more sense than the periodic table. In the first 2 tabs, the student is manipulating EN. In the last tab, we're giving them some real molecules, so it makes sense to give them some real EN values.

As for putting the EN values directly on the atoms... I prefer the table, for 3 reasons: (1) The

table shows EN values for all of the atoms that we're using, not just the atoms in the displayed molecule, so there is opportunity for comparison. (2) Atoms are currently labeled with their element name and partial charge value (possibly adding units), and it's visually cluttered. Adding something else to the atom labels will make this worse. (3) Atom labeling is currently handled by Jmol, since it knows about atom names and partial charges. EN is not something that Jmol knows about - there is no EN atom property, and EN values are not in the mol2 files. So I'd need to take control of the Jmol labels, and generate them for each atom. Any additional Jmol code should be approached with caution, since it is significantly more difficult to write, debug, test and maintain.

CM: Kelly's EN table is directly related to the learning goals of the sim, and ties in nicely with the first 2 tabs. It makes sense to show real EN values for real atoms.

I see nothing in the learning goals about correlating bond type and location in the periodic table. So this Periodic Table smells like a tangent. And in the interest of preventing feature creep, we should take a close look at (a) whether this goal is necessary, and (b) whether the design supports this goal. I'll leave (a) up to you folks. But the current design does not support such a correlation. In the 3rd tab, we are not indicating whether the bonds are covalent or iconic. The 1st tab showed no values for EN, and neither does the 3rd tab, so I don't see how users can possibly determine whether the bonds displayed by Jmol are covalent or ionic. And if they can't determine that, how can they possibly make a correlation to location in the periodic table?

JC: I agree with Kelly's EN table being more directly related to the sim's topic and primary goals, I like what it does, and I think it is better than putting EN values on the atoms (too cluttered).

Chris or Kelly, what do I need to run in the Jmol script in the developer version to change the electrostatic potential color scheme from RWB to the "rainbow" representation we had back in version 0.00.02? It would be helpful for me to be able to compare different color schemes side by side to help me see the benefits of our different choices.

CM: Rainbow color scheme:
isosurface resolution 6 solvent map mep translucent

08/17/11 - Versions 10-11

CM: http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.10/

Lots of progress today on the "Three Atoms" tab, so I'll probably use this version in tomorrow's Chem meeting.

Changes in the "Three Atoms" tab:
- molecular dipole is shown
- bond angles can be manipulated
- molecular dipole aligns with E-field

- added a "rotate molecule" cursor, for discussion

KL: Wow, it's fun to change the bond angle! Can you make it so the atom you are manipulating is always in front? And only have the molecular dipole on by default?

I like how the molecule aligns with the field *after* you change the bond angle. Can you do the same for when you change the electronegativity?

I like the idea of a "rotate" cursor, but it looks pixelated on my computer (and I can't take a screenshot of my mouse).

Julia: you can also use "isosurface VDW map MEP translucent" for the script; the default color scheme is rainbow.

CM: The current image [of cursor] is a rough placeholder. If you like it, we'll create a polished image.

<u>Notes from dev meeting</u>
- CM: how to align Jmol dipole w/ field?
- KL: do we need surface in first 2 tabs?

<u>Notes from chem meeting</u>
Isosurfaces:
- KP: will students relate change in color to electron density shift?
- JC: need a color key for pos/neg potential
- EM: electrostatic potential gives idea of pos&neg, not just electrons
- KL: will students think electron density = atom size?
- JC: rainbow is normal rep, more visually engaging, but complicated; add option for teachers to use rainbow in 3rd tab only
- CM: do not color plates?

Other:
- use new image for PT
- no units on partial charge
- KP: put dipole above or on bond?

CM: In Molecule Polarity, do you want Reset All to request confirmation?

KL: I think the confirmation dialog is unnecessary in this sim. Do you agree?

Also, we should probably not color the plates red and blue for positive and negative. Can you make the plates "glow" instead? Or use some other visual cue when the E-field is turned on?

CM: I agree, confirmation is not necessary. There's nothing vital or time-consuming that they're going to lose by unintentionally pressing Reset All.

Will making the plates instantly brighter suffice? Or does "glow" require additional behavior?

KL: Try brighter for now.

KL: This website has a nice explanation of electrostatic potential maps:
http://people.reed.edu/~alan/ACS97/elpot.html

I attached images of possible color keys for the isosurfaces.

CM: When "Option->Rainbow Electrostatic Potential" is checked, we'll be showing a rainbow spectrum. I assume the labels will be the same as BWR.
Does the midpoint of these spectrum need to be labeled? We discussed how grey (or green, in the case of rainbow) denotes "neutral".

KL: Yes, the rainbow spectrum will have the same labels. I do not think we need to label the midpoint, since the key already indicates "middle." But since Julia requested this feature, let's ask her!

CM: I was asking about midpoint labels in general, not just for the rainbow color scheme.
But it seems especially relevant for rainbow since "neutral" is green.

JC: My 2 cents: I think the same labels for positive and negative will work fine for the rainbow key, same as the RWB one, with no need to label the neutral/middle area.

KL: Here are some thoughts on the startup states of the tabs:

Two Atoms: Move B slider to the middle. That way if students use the A slider first, they see the dipole change direction.
Three Atoms: Again, B slider in the middle.
Real Molecules: Make HF the default molecule. H2 is not very interesting.

We should probably get rid of CO, since it could be confusing.

CM: Got it. I've done all of these, will appear in next dev version.

CM: http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.11/

This version contains a bunch of changes that were requested in the past 24 hours:

- when changing bond angle, move the atom that's being dragged to the front
- pause animation of E-field alignment while an EN slider is being dragged
- make the E-field plates brighter gray to indicate "on", instead of using red/blue
- initialize EN slider for atom B to middle value in all tabs
- use HF as the default real molecule
- remove CO from real molecules, since it could be confusing
- make "molecular dipole" on by default, "bond dipole" off by default in "Three Atoms" tab
- change "Isosurface" label to "Surface"
- disable confirmation dialog for "Reset All" feature
- delete periodic table, replace with a placeholder for electronegativity table
- new rotate cursor, created by Noah P

Electronegativity table and color-key for surfaces coming soon...

KL: Thanks for the quick changes!
- The rotate cursor still looks pixelated on my computer.
- The atom labels are no longer on by default in the 3rd tab.

CM: Rotate cursor is still "in progress". Noah P created the new image, and I've asked him to improve the stroke definition.

Sorry about the atom labels, good catch. I made a major change to how defaults were specified in general (to make them easier to change), and I missed that one. Trivial fix, done and will appear in next dev version.

CM: When we had the periodic table, you mentioned that a View check box would be nice, so that it was initially hidden.
Now that the periodic table has been replaced with the EN table...
Is there any reason to have such a check box for the EN table, or is it OK to display it all the time?
I think it's fine to show all the time, but figured I'd check.

KL: I think we still need the option to hide it.

CM: On or off by default?
And what do you want the check box to be labeled? Electronegativity Table?

KL: Try on by default for now, and label the checkbox “Atom Electronegativities”

TL: I showed this sim to the other chem teachers at my school today and we projected it. They really like the options and we were in consensus that the black and white version would be

better for our students than the multi-color. I just asked them which options they thought they would use- they said the electron density view with the molecular dipole turn on looked most useful.

08/17/11 - Versions 12-17

CM: http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.12/

Changes:
- removed Periodic Table
- added Electronegativity Table, with "View" check box
- added color keys for surfaces
- added "rainbow" color scheme to Options menu
- moved Bond Type indicator near EN sliders, since they are related, and to make room for surface color key
- improved rotate cursor
- fixed default setting in "Real Molecules" tab

CM: I feel pretty strongly that white is not a good background color for the Molecule Polarity sim. White is definitely not a neutral color in this sim. We're using white in many important places in our representations: H atom color, surface color keys, EN table highlighting,... And I think those things are not "popping" as much as they should be. Other problems that the white background is causing include: specular highlights on 2D atoms are washed out; E-field plates don't "glow" as nicely as they could; greater potential for user eye fatigue (I'm definitely feeling it.)

Here's a version with an alternative neutral background:
http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.13/

This version is identical to 0.00.12, with one additional exception: Because the play area is not white, I was able to use better colors for the E-field plates, and I think this "glow" looks much better than the colors I had to use to make this work on a white background.

KL: On my computer, the background colors in versions 12 and 13 look identical.

CM: Version 12 and 13 are indeed different (I just checked), so I guess I chose a color that was too subtle for your graphics display (pale blue, RBG=234,246,255).
Here it is again using the light blue used for the selected tab (RGB=180,205,255):
http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.13/
Hopefully this doesn't display as white on your computer.
I don't feel strongly about this specific color (though I think it works), just that the color should be neutral and not conflict with our representational uses of white and gray.

KL: I definitely see the background color now. I liked how the white background made the sim feel "clean" and made the atoms pop, but I understand the problems with white. By the same

token, maybe we should use pale yellow instead of white to indicate that the electric field is on.

Now that I see the "atom electronegativities" view in the sim, I think it would be better if it was off by default. (And it could go above "atom labels" in the "view" box.) In that case, since students would have to choose to select this view in the control panel, can we get rid of the label in the play area? And the same for the surface color keys? The play area is starting to feel wordy to me.

I also find the color keys to be a bit distracting, but I'm not sure what to do about it. And the rainbow color key should end at blue, not violet.

I'll send this to the chemistry advisory board for feedback tomorrow.

CM: All requested changes are implemented here:
http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.14/

Do you think we're done adding/moving things in the play area? If so, I'd like to start cleaning up the play area layout, to address the type of problem that Trish reported (things getting cropped).

- E-field "on" changed to pale yellow. If this isn't pale enough, please provide RGB values.
- Check box relocated and "off" by default.
- I've removed the labels, but I'm not sold on this, here's why: Start by determining if the representation would need a title in general case. That is, if it had no visibility control (check box), would it need a title? (The answer is "yes" for the representations we're discussing.) If you want to eliminate the title from a representation, you need to look at how effective the control is as a surrogate title. If the control and representation are co-located, the control will probably be an effective title. If they're not co-located (which they aren't in this sim), then users are much less likely to retain the connection between the control and the representation, so the control is less effective as a title. The more representations that are visible (lots in this sim), the more difficult it is for users to retain this connection, and the less effective the control is as a title. For example, go to Real Molecules and check "electron density" and "atom electronegativities", then play with some of the other controls. Now look at the white-to-grey color key with "less" and "more" labels. Less and more of what?... And what are the numbers below the element names in the thing at the bottom of the play area?... Titles on these representations would prevent this disconnect. Or maybe we should consider co-locating the controls with the representations?
- Changed to a linear gradient of (left to right) blue, green, yellow, orange, red. But I thought "green" was neutral and should therefore appear in the middle of the spectrum? See for example H2 or CH4. Something doesn't look right here...

KL: I hope we're done adding things, but I can't say for sure that we won't move things around.

I actually think the yellow on the plates could be bolder.

I'll defer to your opinion on the labels. (So you can add them back.) But can you un-bold the titles? And to be consistent, we should add a label for "bond type."

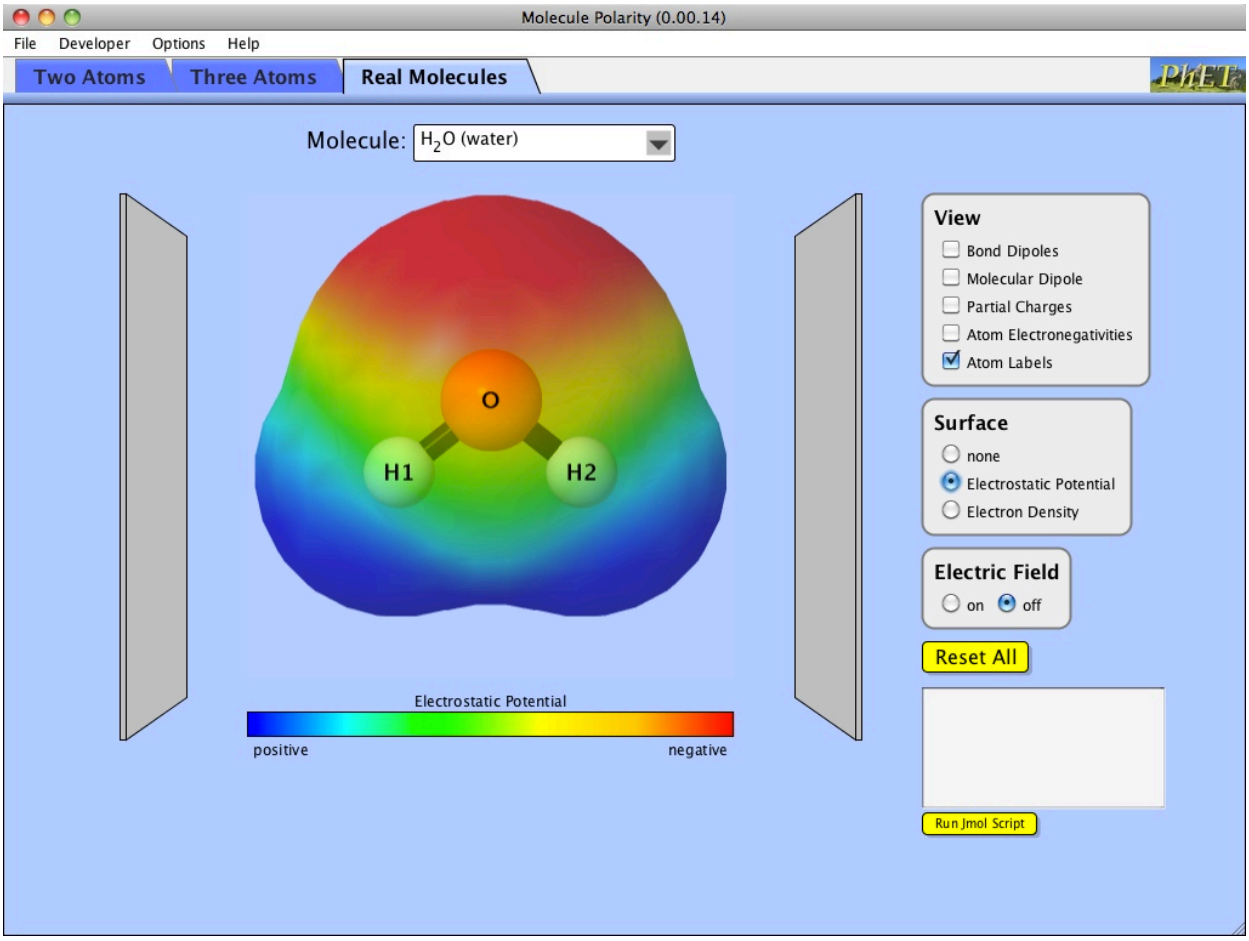
If you look at the electrostatic potential for H2O, you can see a cyan region between blue and green. How does it look if you add that to the color key?

CM: Please send RGB values you'd like for plates. I have a slight concern that this yellow may be confused with yellow in "rainbow" mep color scheme, but since that color scheme is optional maybe we shouldn't worry about it. And yellow sort of makes the plates look "hotter" (to me, anyway).

As for the rainbow color scheme... I do see cyan in the H2O mep. But I don't see any cyan mentioned in the Jmol docs.
Documentation for isosurface command discussion of color schemes shows: "roygb" (default rainbow).
(See http://chemapps.stolaf.edu/jmol/docs/#isosurface)
Jmol documentation on color gradients shows: Direct rainbow (roygb)
(See http://jmol.sourceforge.net/jscolors/#gradnt)

Am I correct that we want green to be in the middle? Adding a single color (eg, cyan) will not shift green to the middle. We'd need to add 2 colors to accomplish that. I'll see what I can come up with...

CM: Screenshots attached showing rainbow color key (after adding cyan) with H2O and H2. Does this look correct?



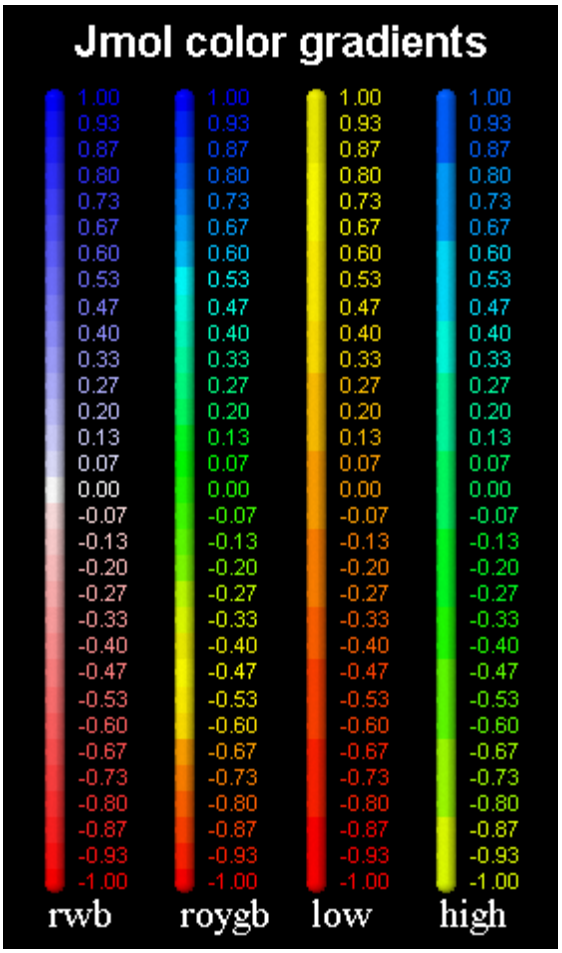
CM: Wanted to check in with you on one feature before I implement it. My "to do" list still contains this:
> Add ruler-like tick marks to EN sliders, make slider snap to closest tick when released.

This feature allows the user to set multiple EN sliders to identical values. Just checking to make sure this feature is still desired. It's non-trivial because we're not using a custom Piccolo slider instead of a Java Swing slider.

KL: Yes, we should include a way for students to compare values on the sliders. I think the EN values could range from 2.0 to 4.0, since that is the range we are using for the “real molecules.” And that range would make it easier to add tick marks.

In the next version, can you try *no* color change for the electric plates? I’m curious to see how it would look.

In the link you sent about the Jmol color gradients, it looks like Jmol does not give equal weight to the colors in the “roygb” scheme. The blue extends to about 0.20, and the color at 0.00 is green.



CM: Here's a dev version with all the changes we discussed:

http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.16/

Changes:
- remove arrows from continuum titles (Bond Type, color keys)
- remove Surface control panel from "Three Atoms" tab
- change EN range to 2.0-4.0
- make Jmol atom labels be hidden by things in front of them
- use 31 colors for rainbow gradient, as shown for "Jmol roygb" at http://jmol.sourceforge.net/jscolors/#gradnt
- use neutral green (0.0 in the roygb gradient) for homogenous diatomic molecules
- remove "more" from range labels on Bond Type indicator
- redesign the Bond Type indicator

I deviated a bit from our discussion about the new Bond Type indicator design. I did implement the "dual triangles" pointer, but it sure looked boring. So I tried something else, a small vertical bond that serves as the pointer. If you hate it, it's easy to revert to the boring triangles :-)

I have not implemented the 2D isosurface in "Two Atoms", or the partial charge for atom B in "Three Atoms". Those are on my list for after lunch.

KL: Looks good! The new Bond Type indicator is definitely better. Let's see what the team thinks.
CM: Glad you like it. Next dev version will go to the team.

CM: http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.17/

Major changes:
- redesigned Bond Type indicator and moved it closer to EN sliders
- added tick marks to EN sliders, with "snap to tick" behavior
- added color keys for surfaces
- added table of electronegativity values
- added "rainbow" color scheme to Options menu
- added partial charge for atom B in "Three Atoms" tab
- removed Surfaces features from "Three Atoms" tab (surface shape is impossible to define, learning goal is satisfied by other 2 tabs)
- no change to color of E-field plates when toggled on/off (using color is confusing and misleading)
- changed bond color to dark gray, so that overlapping black text is still somewhat readable

Missing features:
- Two Atoms: surface shape is incorrect, and coloring is not implemented
- Real Molecules: molecular dipole does not align with E-field

Known problems:
- rotate cursor looks awful on Windows and has been temporarily replaced with hand cursor
- labels on some check boxes are clipped on Mac due to a common-code problem with PSwing
- play area layout needs a bit of polishing

Unresolved design issues:
- location of bond dipoles relative to bonds
- location of molecular dipoles relative to molecules
- better label for "Electron Density"
- final set of real molecules

08/27/11 - Advisory board feedback

(CM: My thoughts on feedback are interspersed below.)

KL: I showed the Molecule Polarity sim in my talk last Thursday and got a lot of feedback from the audience. In short, the chemists did not like that you can change the electronegativity of an atom.

CM: A bit disconcerting, since this is part of the design's foundation... Any idea why they didn't like being able to change EN? Did they not understand that they are changing "customizable" atoms? Or did they not like the fact that polarity is a function of more than just EN?

KL: I also noticed that the signs of the partial charges in the first 2 tabs are flipped - funny that I only noticed during my talk! I also heard from 2 members of the chem advisory board (see below).

JB: Molecule Polarity (0.00.17)
Mac OX X 10.5.8
Java 1.5.0_26

Two Atoms Tab
1) It might be hard for students to figure out that the electric field does something in this tab. Maybe when it initially appears it can be top/bottom so that no matter what the dipole is it will rotate. As it is now they would have had to figure out that it will not move until it is reversed. This discovery will also have to be correlated to actually having the field turned on.

CM: I think he's right -- we should have a different initial orientation so that turning on E-field is more likely to do something. Either flip the EN values for atoms A and B (1 minute), or swap the polarity of the E-field plates (15 minutes).
... or change the initial orientation of the molecule, e.g. A directly above B. (2 minutes to change)
KL: I'd rather not change the initial orientation of the molecule, because I like how it is parallel to the EN sliders. Let's see what students do in the first couple of interviews, and then we can try one of your other ideas.

2) Are the electrostatic potential and electron density features partially disabled? The grey outline appears no matter which is selected and neither changes with various EN configurations. I like this feature if these start working.
3) Are you concerned that the model shows a stick (covalent bond) between the atoms at all times? I know that this is just what the molecular model outputs are, but, we teach that the line represents "shared" electrons. When either surface is selected, will this confuse students?

CM: I have no opinion on this, but changing representations would be a big deal at this point. Your thoughts?...

Three Atoms Tab
1) Here I like that the initial dipole is not in-line with the field and it rotates when you turn it on. I would like to see this same thing as the default setting on the first tab.
2) I was just thinking that it would be nice if you could change the bond angle, low and behold you can! I like this!!!! Should there be some sort of flag informing students of this? Or possibly an angle control up top?

CM: I don't like the idea of angle controls, more clutter and complexity. It sounds like Jack

found this feature quickly, so let's see how this goes in interviews.

3) The partial charges get VERY small, if they are like this when the feature is activated, students might not notice one. Just a thought.

CM: The only way around this is to make partial charges scale nonlinearly, and I think that would be a mistake, it sends the wrong message about the relationship between EN and partial charge. I would wait to see if this is a problem in interviews. If it is, then we'll need to use something other than size to indicate the amount of partial charge.

Real Molecules Tab
1) I like the ability to see the EN values.
2) Is the electric field functional on this tab? Not all molecules are aligned and none move back if rotated.
3) Should there be a call out informing the students that the can rotate the molecule in 3D space? Ones who have never seen this before may not even think this is possible.

CM: Since students will be manipulating the molecules in the first 2 tabs, I don't see any reason why they won't try to do the same in the 3rd tab. Something to watch for in interviews, but I don't think we should do anything now.

4) This tab would be the start for a great VSEPR and Molecular Geometry sim!

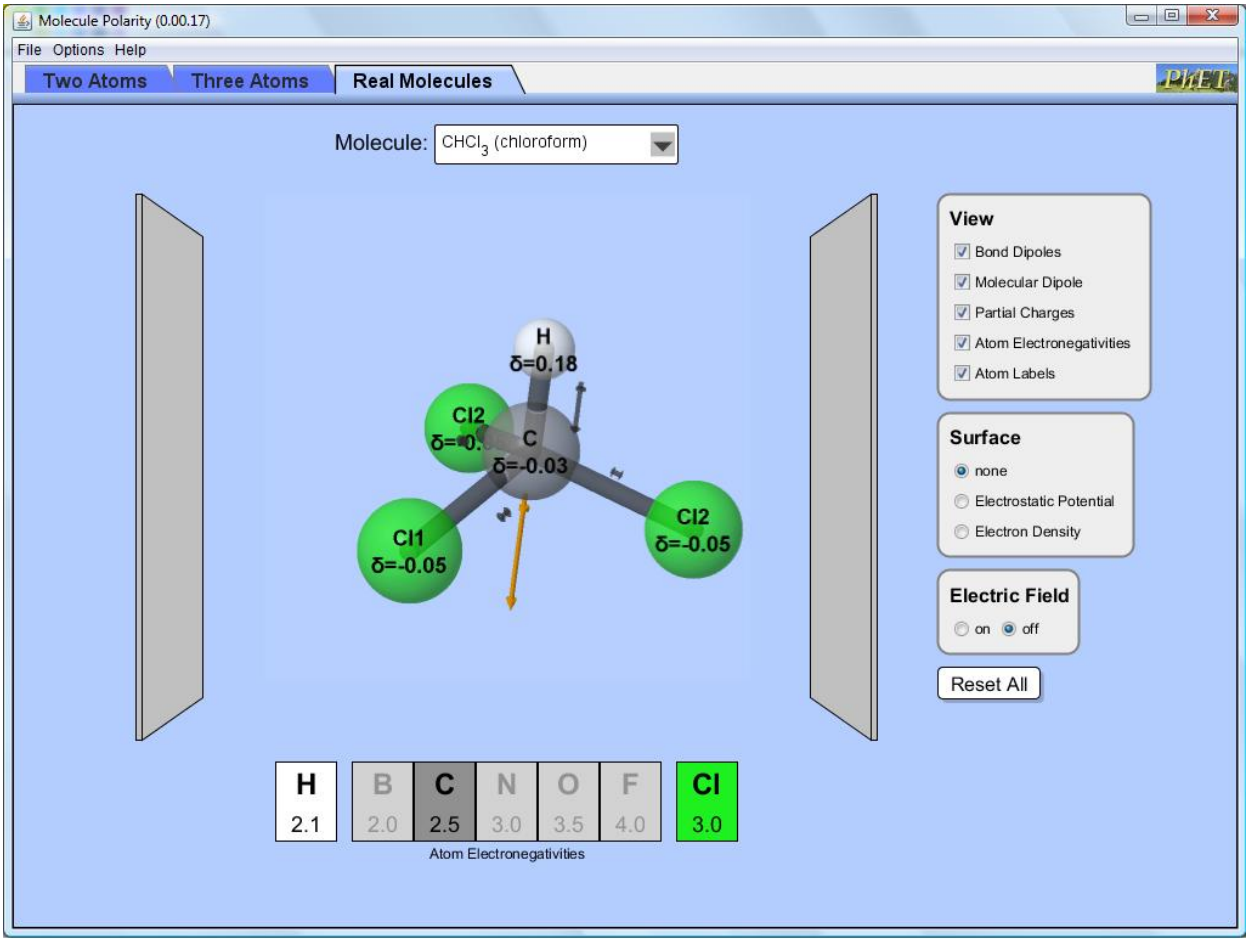
Overall I think the features incorporated would be great for a college-level general chemistry course. The features nicely show things usually represented by static pictures. The ability to drag sliders and witness the change will provide great learning opportunities. Nice work.

KL: Thanks again for the feedback! I copied Chris, who is developing this sim. You found the 2 features that are not yet implemented: the surfaces in the first tab, and the E-field alignment in the 3rd tab. And your other questions are ones we hope interviews will inform.

Emily Moore is actually working on a 3D Molecule Shapes sim. Here is a link:
http://www.colorado.edu/physics/phet/dev/molecule-shapes/

CM: Let me know if you want any changes as the result of this feedback.

MC: I like the molecule polarity one a lot - its something that students do have a hard time with - and I would use this in my class.
I do think that as you get to "real molecules" some of the visualizations are getting pretty hard to make sense of - see attached.



CM: I don't find this piece of feedback to be very useful. Yes, it does look cluttered when you turn everything on at once. But presumably you're not going to do that immediately, and you can turn things on/off selectively. What does she suggest to improve this? Are there specific things that she would recommend omitting, or representing differently? Does use of transparency help or hinder the presentation? Etc.

MC: Also I am not sure what the electric field is for?
CM: Does she mean in general, or in the 3rd tab? Perhaps she didn't try it in tab 2, so didn't see any rotation animation. I wouldn't worry about this, I think it will be obvious once it's implemented everywhere.

KL: I am working on the interview protocol/post-test this afternoon, and I will make sure to include those open questions.

KL: (to Melanie) I'm happy that you like the new Molecule Polarity sim! If you do use the sim in your class, can you let us know how it goes?

I agree that the views in the 3rd tab can get pretty confusing if you turn everything on at once. We start the tab with only the atom labels on, and then students can elect to see more views. In

the interviews so far, students get a lot out of rotating the molecule in 3D.

In the first 2 tabs, the molecule aligns when you turn on the electric field. This seems to help students give the dipole vector some meaning.

We are also working on a Molecule Shapes sim that I think you'd like:
http://www.colorado.edu/physics/phet/dev/molecule-shapes/0.00.32/
You can build molecules in 3D!

09/08/11 - Versions 18&19

KL: We are doing 5 interviews on Molecule Polarity this week and next. Can you fix the signs of the partial charges in the first 2 tabs before Friday morning?

How are the surfaces in the first 2 tabs and the E-field alignment in the 3rd tab coming along? I'd really like to have the surfaces implemented in time for the interviews. The E-field alignment can wait. If you can't get those 2 features completed before the interviews, can you take those options out of the sim?

CM: Changing signs of partial charges is trivial, it will be fixed tomorrow.

Surfaces in tab 1 are likely to be ready before Friday. I know how I'm going to do this, it's not terribly difficult, but it is time-consuming. E-field alignment in tab 3 is unlikely to be ready by Friday. I have some ideas about how to do this, but I'm still looking for an approach that is less costly/complicated/ugly.

Yes, I can remove features fairly easily. If not completed, do you want the E-field alignment removed in all tabs, or only the 3rd tab?
KL: Only the 3rd tab. You can remove the plates in the play area and the "electric field" option in the control panel.

We also have several "real" molecules (NH3, CH3F, CHF3, CH2F2, CHCl3) that have lousy initial orientations. Have you decided whether those molecules are going to be kept?
And have you decided on a replacement label for "Electron Density"?
KL: We can discuss more on Thursday, but for now, the real molecules and labels are fine for the interviews.

CM: Sign on partial charges is fixed in this version: http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.18/

CM: Here's a version for tomorrow's interviews:
http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.19/

Changes:

- electron density 2D representation
- electrostatic potential 2D representation
- temporarily removed E-field features in "Real Molecules" tab
- fixed sign of partial charges

If you run the "dev" version, you'll see a red outline around the play area. This is something new that was added to common code, to help in debugging play area layout issues. Ignore it, it doesn't appear in "production" versions.

09/09/11 - Interview feedback

CM: About the E-field feature for real molecules in Molecule Polarity...

Jmol's scripting language doesn't provide a way to interrogate Jmol about dipoles.
So it's looking like we'll need to read the mol2 file and compute the molecular dipole ourselves.
I'm hoping that you can help me determine how do this.
I'll need the magnitude (for animation speed) and orientation (in 3D space) of the dipole.
The magnitude is probably the easy part.

Attached is a sample mol2 file, for purposes of discussion.

KL: Based on the first 2 interviews (the 3rd student never showed), I am starting to think we don't need the E-field alignment in the 3rd tab. The ability to rotate the molecule in 3D seems to be enough.

KL: Can you move the bond dipoles closer to the bonds in the 1st and 2nd tabs? The molecular dipole in the 2nd tab is fine where it is.

Can we change the cursor for the A and C atoms in the 2nd tab? Or use some other indication that you can change the angle?

If we still want to remove some of the molecules in the 3rd tab, we should consider ones where the partial charges do not follow the EN values for the atoms. But I'd like to discuss with the team first.

CM: How much closer (percentage wise) would you like the bond dipoles? Do you want it similar to Jmol look?

Easy to add a different cursor for bond angle, the hard part is coming up with the cursor graphic design. I'll give it some thought.

Keep me posted on which real molecules make the cut.

CM: http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.20/

In this version, the bond dipoles are as close as possible without overlapping the atoms. Perpendicular offset of the dipole from the bond is 55 pixels, previous versions was 75. Let me know if you'd prefer a different value.

CM and KL phone
- remove “bond type” view?
- add arrows to A & C when hover (see laser in Bending Light)
- make Jmol window larger & zoom out (to see dipoles)
- reorient some molecules
- add periodic table to options?

09/13/11 - Versions 21-22

CM: http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.21/

Changes since 0.0.19:
- added indicator arrows (ala Bending Light) to atoms that can be dragged to change bond angle
- swapped EN values in "Two Atoms" tab to increase the probability that turning on the E-field results in animation
- increased the size of the Jmol viewer in "Real Molecules" tab
- scaled the Jmol molecular dipoles by 80%, so that they aren't clipped by the Jmol viewer
- turned off all Jmol mouse action except rotation
- removed E-field feature from "Real Molecules" tab
- made all floating control panels a uniform width
- decreased perpendicular offset of 2D bond dipoles
- cleaned up the layout of all play areas

Known issues:
- indicator arrows don't go away when molecule rotates due to E-field
- initial orientation of NH3, CH3F, CHF3, CH2F2, CHCl3 needs adjusting
- some control labels are clipped on Mac

CM: You'll notice that the behavior of the "bond angle arrows" is different than we discussed. Hiding the arrows when dragging starts felt awkward/confusing. So they currently behave like they do in other sims (eg, Bending Light). I tried to make the arrows look very different from dipoles, so hopefully they won't be confused with dipoles. Let me know how this looks/feels to you.

KL: Thank you for adding the arrows!

I like how the arrows look when you first mouse over A & C. But when I start dragging the atoms, I find that I pay more attention to the arrows than to the molecular dipole. And if you

never move your mouse off A & C, the arrows are always there. How weird/complicated would it be to disable the arrows (for the remainder of sim play) after the student clicks on each atom?
CM: I really dislike feedback that only occurs once. I'll create a version using the behavior that we originally discussed, and see if you like that any better.

I actually prefer the previous setting of the EN sliders. That way, when students use the A slider (which they will almost always do first), they see the dipole change direction. Also, students tend to change the EN values before turning on the E-field.
CM: OK, I'll switch them back.

I like the new size of the Jmol window! But some of the dipoles are very small; the ones in CH2F2 look like dots. Can you make the window even bigger? Also, the window feels too close to the control panels. Can you move the window to the left (or the control panels to the right)?
CM: The dipoles shouldn't be any smaller (relatively) than they were previously. Are you seeing some dipoles that are now smaller?
With the current layout, I can't make the Jmol viewer any bigger. We are limited in the vertical direction. If you want the Jmol window larger, something needs to be moved. For example, we could move the "Molecule" combo box above the other control panels, and that would give us more vertical space.
Yes, I will add some horizontal space between the Jmol viewer and control panel.

I'll see if I can do a couple more interviews early next week. I may ask you to remove the "bond type" view for those interviews.

JC: I also like the arrows to encourage bond angle play. I noticed that when I click and hold to rotate the molecule from the bond and move my mouse over A or C, the angle change arrows appear, even though the rotation function is engaged.

Other small things include that I have a red stripe border around the sim on the blue background on all 3 tabs (I'm running mac 10.6.8; not sure what version of java I have). Also, I can faintly see a color difference between the jmol viewing window in Tab 3 and that tab's background color, but I've never noticed it before and don't think it's problem.

CM: The red outline is something that was added to common code as an aid for debugging layout issues in the play area, it shows the boundary of what we call the "stage", which is the area that's guaranteed to be visible. The red outline appear only in the "dev" version, it does not appear in the "production" version.

The faint color difference has been there for a long long time. The ideal solution would be to make the Jmol viewer background transparent, but that's not supported by Jmol. And Jmol is doing something to muck with the color. So I'm afraid we'll have to live with it.

CM: http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.22/

Changes:
- reverted to original EN values for atoms in "Two Atoms" tab
- added horizontal space between Jmol viewer and control panels in "Real Molecules" tab
- changed initial orientation of NH3, CHCl3, CHF3, CH2F2, CHCl3
- put red outline around stage bounds only for dev versions

CM: I haven't changed the behavior of the bond angle arrows, that's going to take some time. I might not get to it until next Monday.

Please review the initial orientation of all real molecules, check to see that (1) molecule structure is correct, (2) all atoms are visible, and (3) molecular dipole is visible. Awhile ago you sent me screenshots for desired orientations, but some of those hid the molecular dipole, so I improvised.

KL: - initial orientation of real molecules
This looks great! Can you give CHF3 (trifluoromethane) the same orientation as CHCl3 (chloroform)?

- size of dipoles for real molecules
I checked previous versions of the sim, and the dipoles have always looked like dots for CH2F2 (difluoromethane).

CM: Do you want me to do anything about the dipoles for CH2F2? Jmol sizes the dipoles for all molecules relative to their magnitude, so increasing the length of CH2F2 dipoles can only be done by increasing the length of *all* dipoles, or writing some code that does specific scaling for CH2F2 only. Is CH2F2 the only culprit? If so, should we consider dropping it? CHCl3 also has some short dipoles, though not quite as short as CH2F2.
KL: Let's add this to the list of things to consider when we decide on the final list of real molecules.

TL: One comment I have is that the blue background projects very well in my classroom. I have attached a couple of sims on my interactive white board (less reflective than just a screen). The light blue used in Capacitor lab is much more easy to see than the black of the molecule sim. These pics were from the front row, so some students are another 14 ft back.

Just a note as a user - I didn't realize that the molecules were grabbable. I think a note in the Tips would be nice.

CM: I figured out a relatively easy way to scale the dipoles for individual molecules.
The size of dipoles (bond and molecular) within a single molecule would be consistent.
But relative comparison between molecules would no longer be meaningful, because different molecules would be using different dipole scales.

Let me know if you want me to implement this.

KL: I think it's important for the dipole scale *between* molecules to be consistent, so let's not implement this.
CM: OK, that's my feeling, too.

09/19/11 - Version 23

CM: http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.23/

Changes:
- changed behavior of bond angle arrows (visible when mouse enters atom, disappear when mouse exits or when drag starts)
- made CHF3 have same initial orientation as CHCl3
- added rotate cursor to 2D surfaces
- moved Jmol Console (for testing scripts) to Developer menu
- lots of internal cleanup and refactoring

Outstanding design issues, for discussion at Chem meeting:
- better label for "Electron Density"
- should we get rid of Bond Type indicator? (tangential, confusing in interviews, see Jack's ball-and-stick concern)
- Jack: concern about showing ball-and-stick representation at all times? (address by dropping Bond Type indicator?)
- Jack: partial charges are sometimes very small, will students see them?
- is E-field feature necessary in "Real Molecules" tab?
- CH2F2 and CHCl3 have tiny bond dipoles, is this an issue?
- what is the final set of molecules?

KL: I like the new behavior of the bond angle arrows. I also have an interview at 11am today. Can you hide the "Bond Type" indicator before then?

CM: Bond Type feature is hidden in http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.24/

CM: In the View panel, would you mind if I moved the "Molecular Dipole" check box above the "Bond Dipoles" check box? When going from "Two Atoms" to "Three Atoms", it feels odd to have the new check box appear between the "Bond Dipoles" and "Partial Charges" check boxes.
KL: I think the order we have it in now makes the most sense conceptually. But we can add this to the list of things to discuss at the chem meeting on Thursday.
CM: We have bigger fish to fry, so probably not worth discussing.

09/22/11 - Versions 24-26

CM: Lastest dev version:
http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.24/

Outstanding design issues:
- better label for "Electron Density"
- should we get rid of Bond Type indicator? (tangential, confusing in interviews, see Jack's ball-and-stick concern)
- Jack: concern about showing ball-and-stick representation at all times? (address by dropping Bond Type indicator?)
- Jack: partial charges are sometimes very small, will students see them?
- is E-field feature necessary in "Real Molecules" tab?
- CH2F2 and CHCl3 have tiny bond dipoles
- final set of molecules
- layout change in "Real Molecules" to allow making Jmol viewer bigger
- larger font for controls

Notes from chem meeting
Remove bond type indicator?
- KP & TL want to address learning goal: ionic vs. covalent
- KL & JC: already in Sugar & Salt sim
- KP: or relabel as more/less covalent
- CM: move to options menu?
- KP: how to make it not look like slider?
- RP: vertical bar graph of “ionic character”
- JC: horizontal graph of “bond character”: covalent = color A, ionic = color B
- KP: not cross over whole slider (horizontal bond)
Other
- add icons to dipoles, make font bigger
- for teacher’s tips: in 3rd tab, charges do not always follow EN

CM: I remembered another reason why we dropped the dipole icons next to the check boxes: dipoles looks slightly different in different tabs (2D vs 3D). And while I control the drawing of 2D dipoles, I don't have a way of getting Jmol to generate dipole icons.

Options, in order of decreasing cost:

(a) Create a 3D dipole icon in Photoshop or Illustrator, and use it in "Real Molecules". This creates a potential maintenance issue if we ever change the look of Jmol dipoles. (Cost = 2-4 hours)
(b) Use the 2D dipole icons in all tabs. This will emphasize a difference that is otherwise subtle. (Cost = 1-2 hours)
(c) Don't add the icons. Lack of icons didn't seem to be an issue in interviews, and provides more space for translations. (Cost = 0)

Which option would you prefer?

CM: http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.25/

Changes:
- redesigned "Bond Character" indicator
- increased font size in control panels
- workaround for difference between background color of play area and Jmol viewer
- workaround for PSwing clipping of control labels on Mac
- vertically centered molecules between E-field plates (they were slightly off center)

I have not added icons next to dipole check boxes (see previous email which enumerates the options.)

The new "Bond Character" indicator seems like it has all of the same problems as the previous design. I think the difference between "type" and "character" will be lost on students, the term "character" is likely more foreign/intimidating, and I suspect that they'll still try to drag the tiny molecule. The tiny molecule also looks odd without a connecting bond. Imho, this sim would be better served by dropping this feature, and addressing bond type in a future sim.

JC: I really like the new bond type indicator, and I am in favor of leaving this feature in, since different types of bonding are a difficult topic to address in any sim. I think the changes help it look less like a slider.

The other changes are great--I noticed the background color looks good!

As for the icons options, clearly the sim works without them, but I don't think there would be a big problem with having slightly mis-matched arrows in the 3rd tab. So, my vote is for little arrow icons for bond dipole and molecular dipole in each tab, in 2-D. Option B, in Chris' list.

CM: All votes were for (b), so I'm proceeding with that option.

CM: http://www.colorado.edu/physics/phet/dev/molecule-polarity/0.00.26/

Changes:
- added icons next to dipole check boxes
- tweaked layout of "Three Atoms" play area to leave room for control panel translations
- added bond to tiny atom in Bond Character indicator
- many internal changes in preparation for code review

All features and change requests have been implemented.
This version is a 1.00 release candidate, so please test it thoroughly.

JC: This is really nice. I tried all the features out, and I think it's ready for the deployment!
KL: The only things I saw were typos in the Credits.

KP: Looks great to me. I could also be happy if the labels on the bond character indicator were 2 lines and said “more covalent” and “more ionic” if that seems better to Kelly or other team members.

I played with it for a little while and didn't find any bugs. One super-small thing, which is fine to leave, but I just saw it so I'm putting it out there ... the check-boxes got a bit misaligned with addition of the image.

Website

Main Topics
polarity, electronegativity

Keywords
molecule, polarity, atom, electronegativity, bond, dipole, partial charge, surface, electrostatic potential, electron density, electric field, covalent, ionic

Categories
new sims, chemistry, general chemistry, high school, university, (biology?)

Credits (check in sim also)

- design team
Kelly Lancaster (lead)
Chris Malley (developer)
Julia Chamberlain
Emily Moore
Robert Parson
Kathy Perkins

- third-party libraries
Jmol, (Spartan?)

- thanks to
Jack Barbera, Trent Parker

Description
(write)

Learning Goals

(copy)

Teacher's Guide
(write)

Related Sims
Molecule Shapes (Build a Molecule, Molecules & Light?)

Teaching Ideas
(upload gen chem activity)