Build a Molecule

Post your ideas for the title here:
molecule maker
molecule construction kit
molecule factory
molecule master
molecular monarch
molecule workbench
molecule constructor
making molecules
simple molecules
molecule builder

PhET Sim Design Document

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Public URL:
https://docs.google.com/document/pub?id=1MPBZ6L-a1j6SX7ZWQt1u1SUFbjROQTyuQUDsMyBX7F0

Abstract:
What's the difference between atoms and molecules? Molecules are made of atoms.
Starting from atoms/elements, build some common molecules.

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Audience

This sim is primarily intended for use by middle school students, roughly grade 6 or 7. These students should have some understanding of what atoms are, and would recognize the names of the elements that we use, i.e. oxygen, carbon, hydrogen, and nitrogen. They don't necessarily need to be familiar with the names of some of the compounds that they are likely to create, such as carbon dioxide.

Learning Goals

After using the sim we hope that students are able to:
Basic:

- Describe the differences between an atom and a molecule.
- Construct simple molecules from atoms.

More Challenging:

- Recognize that the subscript in the molecular formula indicates the number of that atom in the molecule, eg. two hydrogens are in the molecule H_2O.
- Recognize that the coefficient indicates the number of molecules, e.g. $2H_2O$.
- Associate common molecule names with multiple representations.

Maybe in later tabs:

- Determine the molecular weight from the sum of the atomic weights? (with introduction of scale feature?)
- Describe common substances as consisting of many individual molecules.
- Have students select elements from the periodic table to build a given 'target' molecule. This might help connect 'element' to 'atom' to 'molecule

This sim will not address:

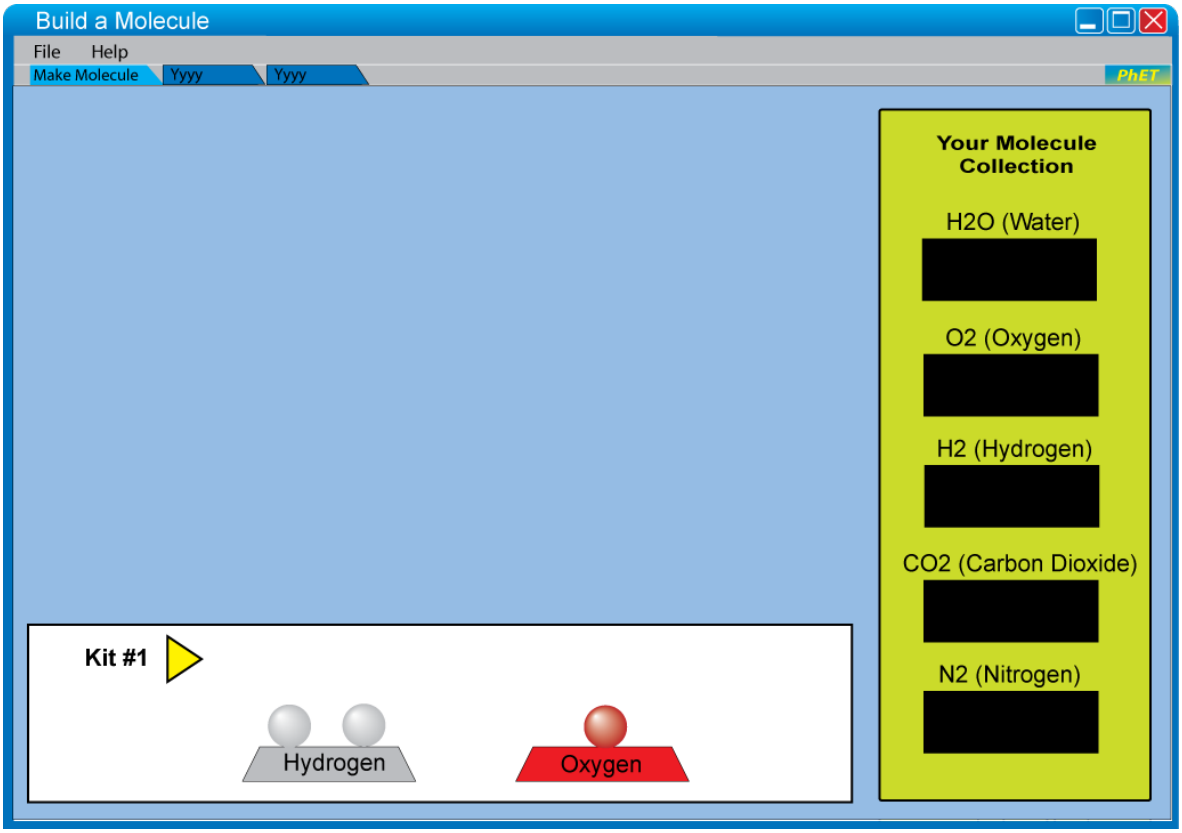
- Bonding in molecules

Additional Requirements

It has been suggested that this simulation be used as a precursor to the Balancing Chemical Equations simulation, since this will help to get students familiar with various molecules before attempting to balance equations that make use of them. For this to work well, the two simulations need to have identical, or at least very similar, representations of the different molecules and atoms.

Mockup

1st Tab - Collect Single



Goal: To build at least one of each of the molecules listed on the right.
Given: A list of molecules to 'collect', and a selection of kits, each containing enough atoms to make one of the molecules to be collected.

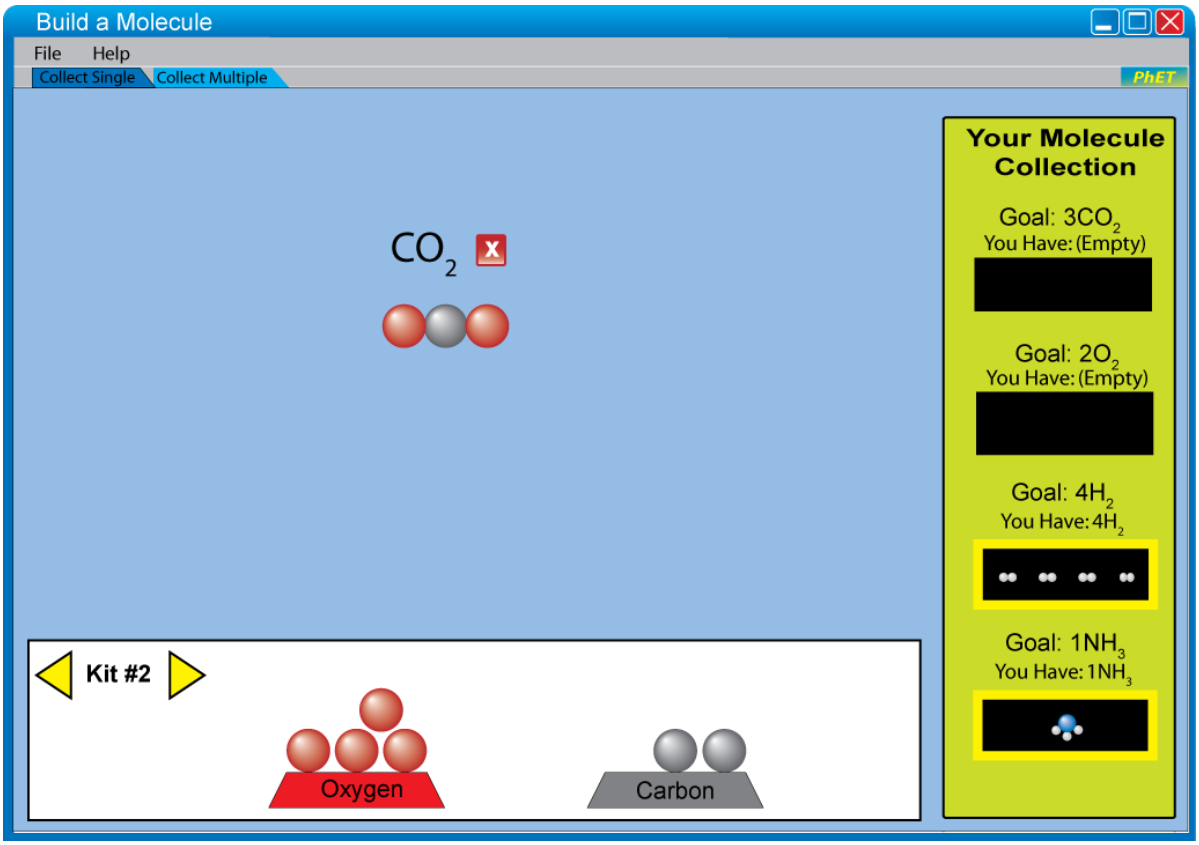
Students choose a kit to build from, and then can drag the atoms into the play area to build the molecules. Once students make a molecule from the list, the molecule will show up in the appropriate collection box.

*You cannot mix atoms from different kits in the play area at the same time.

Once all collection boxes are filled, boxes are highlighted and the student gets an indication that they are done.

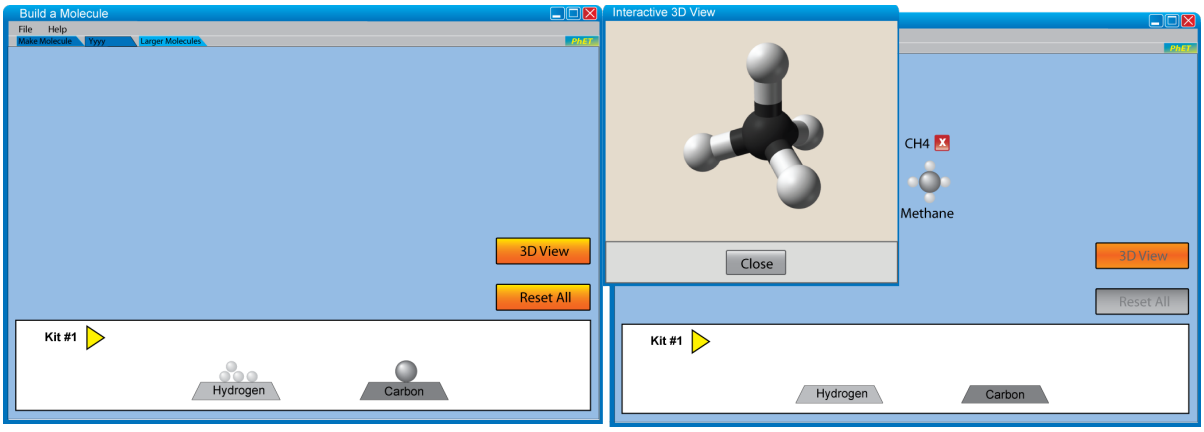
Tab 1 Questions:
JO: Should we then mark that kit as "completed", and/or do we want them to play around with it more?
EM: I don't think the kit should be marked as completed. I think the focus should be more on filling the "Molecule collection" rather than on 'completing kits'.
JO: Should each kit retain its own state? That way, a partially constructed molecule in kit #1 could be seen again after the student switches to other kits.
EM: Yes, each kit should retain it's own state.

2nd Tab - Collect Multiple



Goal: To collect the correct number of each type of molecules listed on the right. Students now need to collect not just a single molecule of type listed in the collection area, but the correct number of molecules. Once a student collects the correct number of molecules, boxes will light up and students get an indication that they've completed this tab, though a new set up goals in the collection area will appear so students can keep playing this tab if they want.

3rd Tab - 3D View

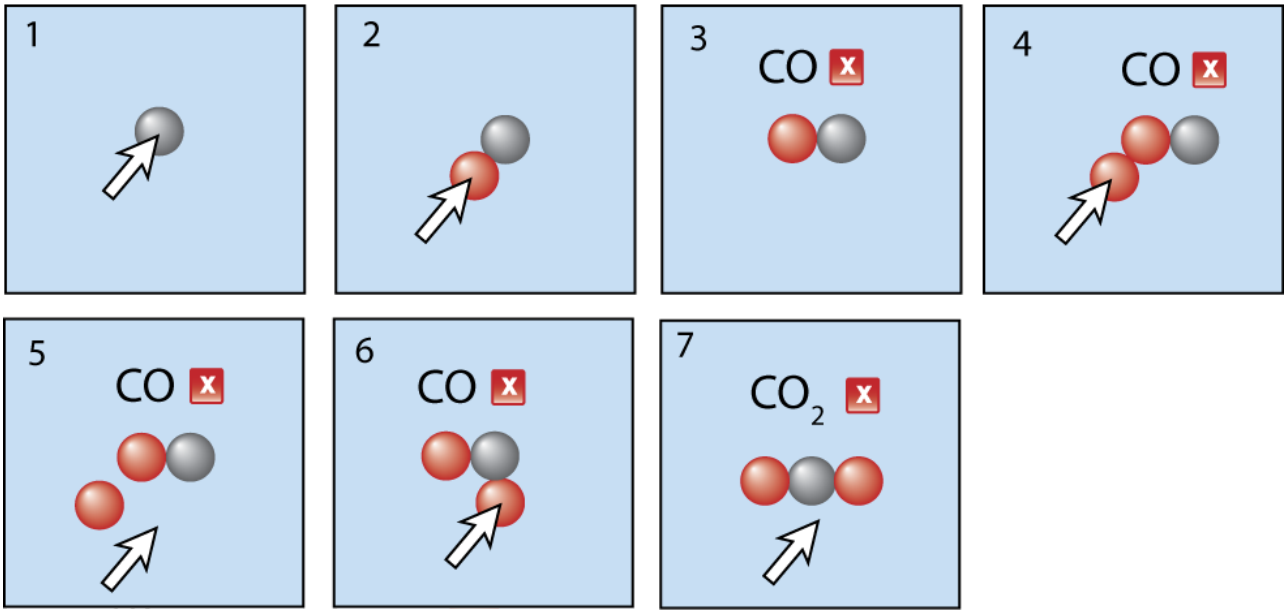


Students will be able to build any molecules they want from a selection of kits. Students have the option of selecting 3D view, and a Jmol popup box will appear, showing the molecule in 3D and allowing for rotations (and changes in representation?).

Interaction of atoms in play area

The use of kits will constrain the number of molecules students can make, by limiting their starting materials. There will be cases, though, where they can make multiple different molecules from the starting materials.

User builds CO_2



In the example above, the student makes a molecule (CO) on the way to making the desired CO2 molecule (presumably the CO2 molecule is needed to fill a collection box).

1) Student drags out an carbon atom.
2) Student drags out oxygen atom.
3) Molecule realigns itself and the name of the molecule appears above.
An ‘X’ box allows the students to dissociate the two atoms, breaking up the molecule.
4) Student drags another oxygen atom to add to the CO molecule, but tries to add in the incorrect structural location.
5) Second oxygen is repelled away from the CO molecule.
6) Student tries to add second oxygen atom to the other side of the molecule.
7) Molecules rearranges slightly to show the correct structure, and the name CO2 appears.

NOTE: For each molecule kit, the various molecule options must be determined and all possible molecule-making scenarios accounted for. It will probably not work to have a single set of atom interaction rules that works for all cases.

Interaction of atoms Questions:

JO: Clarification: for a molecule with 3 or more atoms, only one 'X' is shown that will dissociate all of the atoms?
EM: Yes, only one X for each molecule.

JO: How we determine molecule-making scenarios is a core part to the implementation, and would be very helpful to get hammered out first.
Question 1: Are there "intermediate" forms like possibly NH_2 that are not considered "molecules" under the "electrically balanced" definition that we need to step through? Should we show names, or make a note that these are not considered molecules?
EM: No intermediate arrangements that aren't themselves neutral, (reasonably) stable species will need any indicators (no names, or acknowledgments of non-molecule being-ness). The sim will in no way address how any molecules are actually formed (the goal is only recognition of the molecules made, not understanding of formation), so the presence of intermediates doesn't need to be addressed, and would be a royal pain.
Question 2: If the answer to (1) is yes, do we prevent all intermediate forms that do not lead to a possible molecule?
EM: Arrangements that don't lead to molecules will not be allowed, by way of the repulsion shown in the CO2 example above. That's part of the reason why each kit will have to have a set of rules (which things go where, which things repel in what conditions) that is unique. I'll start this Friday (3/25/2011) working on sets of atoms/molecules for the kits (and rules regarding arrangements and repelling), and run those by a local middle school teacher (Jackie) next week.

Questions:

EM: Perhaps the x button should be a bit smaller, or maybe only appear when they mouse over? I'm concerned that students might start associating the x with the name, but this may not happen during the dynamics of play.
KL: I agree that the "x" button is distracting and it's function is not immediately clear. How about a button that says "Break apart" or something to that effect?

EM: How will the atoms be collected? Dragging over to the collection area, automatically appear in collection area (this will only work if students can drag out of the molecule collection box), or an option to 'save' molecule.
JO: If we show a "tip" the 1st time that says something like "You have just created a molecule. You can drag it over here", that it would work quite well.
EM: I think this is a good idea. What if, the first time a molecule listed in the collection box is made, a pop up appears at the collection box that says something like "Drag your molecule here". As a second option, it might be sufficient if on the first tab, once a molecule is made that is listed in the molecule collection, the appropriate box starts blinking.
JO: Is it bad conceptually to think of the collection area as another "view" of the play area? So whatever molecules are constructed show up both on the play area and in the collection area?
EM: Sometimes molecules can be made that might not be listed in the collection area. I think it makes the most sense to keep the list of different molecule types to be collected on the order of 5 or less, but it's possible that even with a relatively small number of atoms in each kit, more than these 5 molecules can be made. So not all possible molecules will be listed in the collection area. This could also lead to an option of having a new set of collection boxes appear, once all the original collection boxes are filled. With this option, students would have the original set of boxes shown, fill them up, get some indicator that they have done awesome, and then can get a new set of boxes to fill (or move on to the next tab).

EM: I think that once all the atoms for a molecule are put together, the final representation

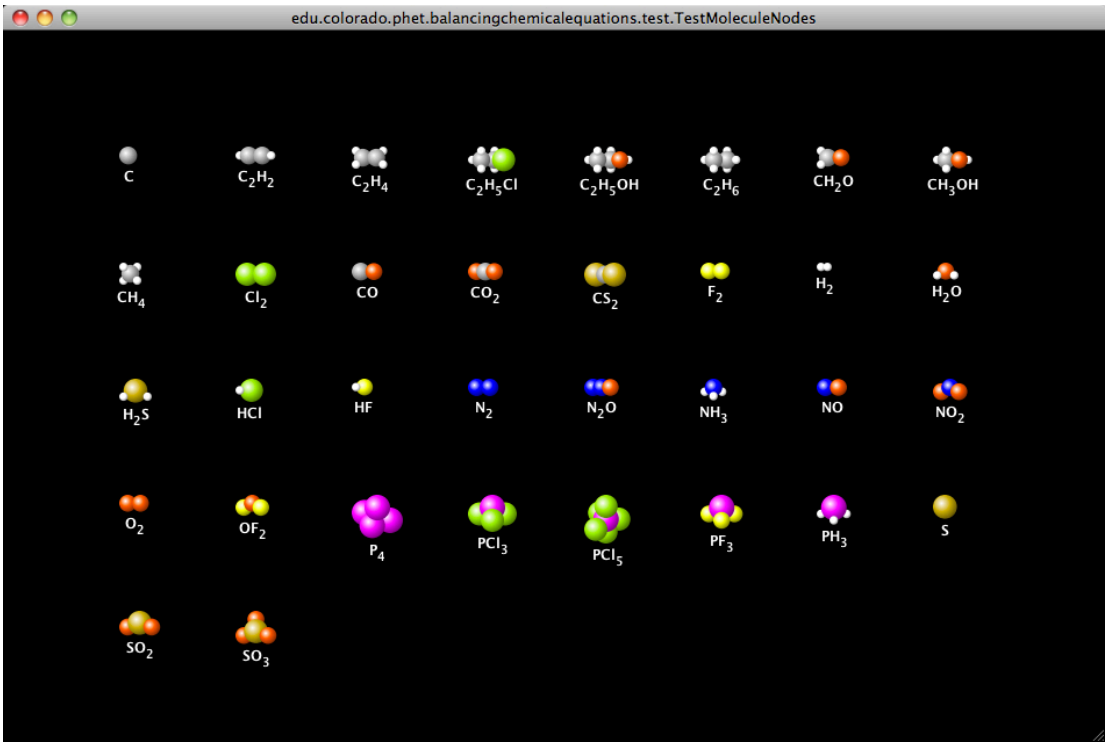
in all tabs in the play area should be at least pseudo-3D (for example, in the methane case of Tab 3 shown above, I think that students should be able to put the hydrogens around the carbon as shown, but once all hydrogens are there, a pseudo-3D image of methane should appear, replacing the more Lewis dot structure type representation.

JO: Is there any way to show it in pseudo-3D while it is being constructed? I could imagine that would be helpful for larger molecules.

EM: Particularly since there will be a set of rules in place regarding all possible combinations, this might not be too difficult. It means atoms will have to rearrange as they're being built.

JO: Also, what should this pseudo-3D view look like?

EM: Below is list of molecules Chris made (in piccolo) for Balancing Chemical Equations. This is what i'm referring to as pseudo-3D. In the case of 2 and 3 atom molecules, the list below shows some overlapping between atoms, for example in Cl2 (second row, second column) where the left atom is slightly behind the right atom. That's not necessary for our purposes, but is fine if it's easier to reuse these images some way. For 4 atom molecules and higher, some atoms in 3D would actually be somewhat behind others so that would need to be shown. Notice, though, in the case of the 6-atom molecule PCl5 (fourth row, fifth column) that it's really difficult to actually see what atoms are present, which is why I mentioned previously that above 5-atom molecules, actual 3D would be better.



Combinations of H, N, O, and C Atoms that form stable (Diatomic or Triatomic) Molecules

In the spreadsheet (BuildAMolecule-Spreadsheet), a list of all possible diatomic and triatomic combinations from the atoms H, C, N and O are listed. All possible stable diatomic and triatomic molecules are named.

Not sure if I should include all possible combinations of four atoms (240 combinations possible).

To Do:
KP: Add symbols to atom ‘balls’.

Questions:
- Button to choose between molecular formula and name?
(1): Should we support showing a "schematic" view in the collection boxes? (possibly hard to see).
If so, should we only show a "canonical" version? Molecules with a vertical layout may be very difficult to see.

(2): Currently the highlight showing a completed collection box is (to my eyes) somewhat faint. Should the colors be changed, and/or should we add in
a sound when a collection box is filled?

(3): Should we add in an indication that a just-created molecule could be put in an associated collection box?

(4): How should resetting work in general? Should we have a "Reset All" button, and should this reset back to the very initial configuration of the
tab like normal? Should we have a "Reset Kit" button that pulls all atoms back to the buckets (and pulls molecules out of collection boxes if
necessary)?

(5): Current behavior when trying to add a molecule to a "full" collection box just pulls it back out to the play area. Is this acceptable?

(6): Current behavior of the molecule readout is in conflict with the design doc. Doc shows "H20" above the molecule in ONE part, and in another
shows the formula above and the molecule name BELOW. Sim shows the molecule name (e.g. "water") above currently, but could easily switch to showing
the formula in addition (additional padding between molecules may be necessary)

(7): For kits and collection boxes (particularly randomly generated ones), is it ok for 1 kit to not completely fill one multiple-molecule collection

box? For instance, if we want 2 C2H2, a kit with four carbons would require MANY more molecules in our database, so we may want to have a larger
quantity of kits than collection boxes.

(8): Is the scale of the pseudo-3d molecules in the collection boxes OK? (We can only fit 2 C02s with the current size, but we could increase the
width of the actual collection boxes a bit safely.

(9): I am not terribly pleased with the spacing on the 2nd tab collection box labels. The subscripts are farther down and larger than shown in the
design doc, so the layout gives it more space. Should we either (a) tweak the subscripts to be smaller, (b) try to manually reduce the padding, or
(c) combine the 1st and 2nd lines somehow, or put the 2nd line to the left of the collection box? We could even put the quantity (e.g. 1NH3) inside
the collection box on the left, and shift the molecules to the right.

(10): For molecular formulas, I was under the impression that the Hill System was the standard, however this gives us "H3N" for "NH3". Is there a
procedure or set of steps that can be used to get an accurate naming convention? (One way that may work would be to break the Hill convention and if
there is no carbon, STILL put the hydrogen first).

(11): We currently have no design for the "You have filled all of your collection boxes. Would you like to fill a different set of collection boxes?"
dialog. Should I add in a prototype, or should we sketch a quick design first?

(12): For the 3rd tab (3D view), it should be possible to change the view style. We could offer the user "Filled spheres", "Ball-and-stick", and
possibly more. Do we want to integrate those style changes into the design, or should I work them into a prototype?

(13): Currently atoms all move with the same speed in different situations (falling back to buckets, moving back to the play area, breaking apart).
I'd like to speed up movement when the atom is far from its destination, but keep it about the same when it is close (like breaking up). Is that OK?

Kit Scenarios:

If we use kits, then there's no reason to restrict the different atom types! This list of molecules includes covalently bonded, neutral molecules that are found commonly in nature, or as examples in chemistry texts.

Two-atom molecules:
Hydrogen (HH)
Oxygen (OO)
Nitrogen (NN)
Fluorine (FF)
Carbon Monoxide (CO)
Nitrogen Monoxide (NO)
Hydrochloric Acid (HCl)
Hydrofluoric Acid (HF)

Three-atom Molecules:
Water (H_2O)
Carbon Dioxide (CO_2)
Trioxygen or Ozone (O_3)
Dinitrogen Monoxide (NNO)
Hydrogen Sulfide (H_2S)
Hydrogen Cyanide (HCN)
Borane (BH_3)

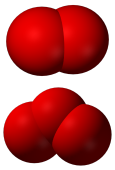
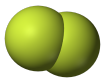
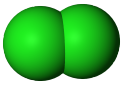
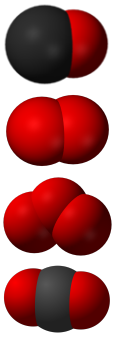
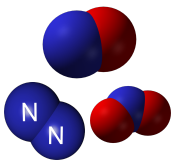
Four-atom Molecules:
Ammonia (NH_3)
Hydrogen Peroxide (H_2O_2)
Acetylene (C_2H_2)
Phosphane (PH_3)
Formaldehyde (CH_2O)
Beryllium Fluoride (BF_3)

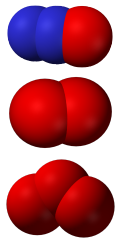
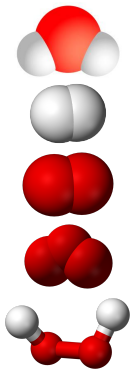
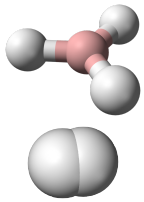
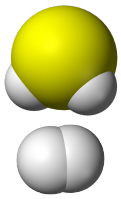
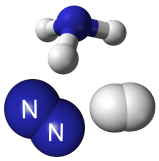
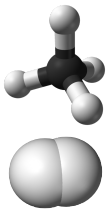
Five-atom Molecules:
Methane (CH_4)
Silane (SiH_4)
Fluoromethane (CH_3F)
Chloromethane (CH_3Cl)

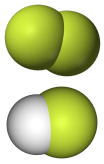
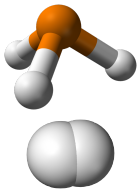
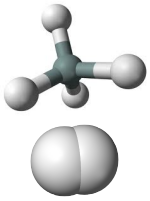
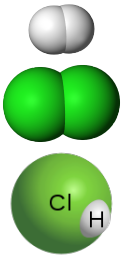
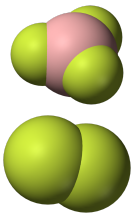
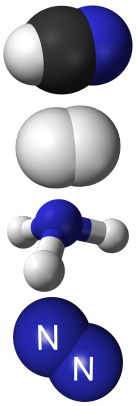
Kit Scenario Specifics:

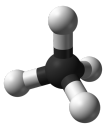
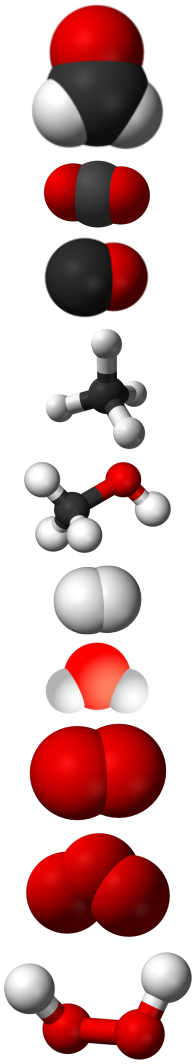
Kit Theme: Atom contents
Issues: how to deal with cases where a not allowed combination of connections is necessary to build molecule? Comes up when not all diatomic combinations allowed that lead to stable triatomics.

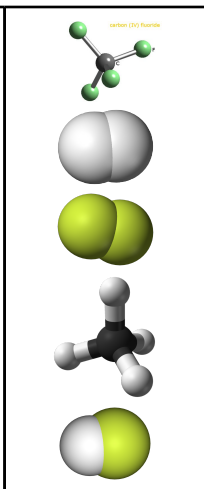
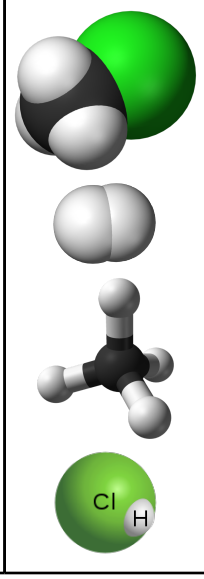
Solution: Have two categories...1) allowed and 2) allowed + molecule

Name	Connectivity	Scenarios	Molecule Images	Molecule Names
Hydrogen	H = 1	- Two together make H2 - no other additions allowed		**H2**
Oxygen	O = 1 or 2	- two together make O2 - addition of a third makes O3		**O2, O3**
Nitrogen	N = 1	- two together make N2 - no other additions allowed		**N2**
Fluorine	F = 1	**-** Two together make F2 - No other additions allowed Fluorine forms 1 connection		**F2**
Chlorine	Cl = 1	- Two together make C2 - No other additions allowed		**Cl2**
Carbon/Oxygen	C = **1**, (never C as connector), **2** O = **1, 2** (if first connection is C, no 2nd connection allowed)	- C and O form CO - Addition of second O allowed on carbon side only, makes CO2 - Two O together form O2 - Addition of third O forms O3 **No Limit on C or H**		**CO, O2, O3, CO2**
Nitrogen/Oxygen	N = **1,2** (if one connection is N, no 2nd connection allowed.) O = **1, 2** (if one connection is N, no 2nd connection allowed)	**No Limit on N or O**		**NO, N2, NO2, N2O, O2, O3**

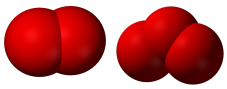
				
Hydrogen/Oxygen	H = 1 O = **1** (if connector H, allowed but not molecule), **2** (if one connector H, another connector as O allowed but not molecule...unless O connector has H connector as in HOOH)	**No Limit on N or O**		**H2O, H2, O2, O3, H2O2**
Hydrogen/Boron	B = 3 (Never B as connector) H =1	**No Limit on B or H**		**BH3, H2**
Hydrogen/Sulfur	S = 2 (Never S as connector) H = 1	**No Limit on S or H**		**H2S, H2**
Hydrogen/Nitrogen	N = **1** (if connection is H, allowed but not molecule), **3** (if first connection N, no other connections allowed) H = 1	**No Limit on N or H**		**NH3, N2, H2**
Hydrogen/Carbon	C = 4 H = 1	**Limit 1 C, No Limit on H**		**CH4, H2**
Hydrogen/Fluorine	H = 1 F = 1	**No Limit on H or F**		

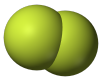
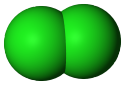
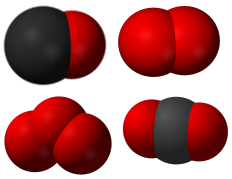
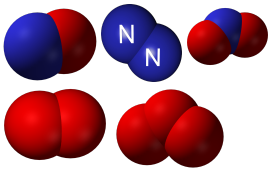
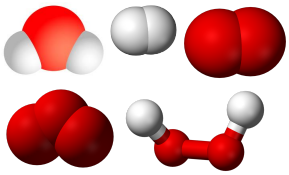
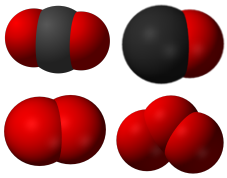
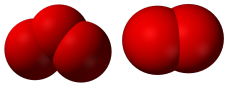
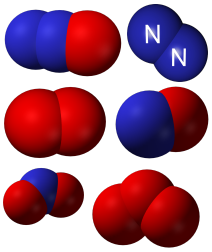
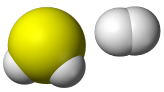
				
Hydrogen/Phosphorus	P = 3 (Never P as connector) H = 1	**Limit 3 P (unless allow for P4), No Limit on H**		**PH3, H2**
Hydrogen/Silicon	Si = 4 (Never Si as connector) H = 1	**No Limit on Si or H**		**SiH4, H2**
Hydrogen/Chlorine	H = 1 Cl = 1	**No Limit on H or Cl**		
Boron/Fluorine	B = 3 (Never B as connector) F = 1	**No Limit on B or F**		**BF3, F2**
Hydrogen/Carbon/Nitrogen	H = 1 C = **2** (never C as connector, if one connector N only one H allowed as another connector), **4** (Never C as connector, Never N as connector...this means once N is connected only 2 total connections allowed) N = **1** (connection to H or C allowed, but not molecule), **3** (Once N or C connected only 1 total connection allowed, if first connector is H then only 3 total H connections allowed.)			**HCN, H2, NH3, N2, CH4**

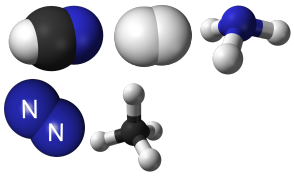
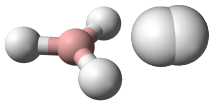
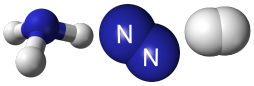
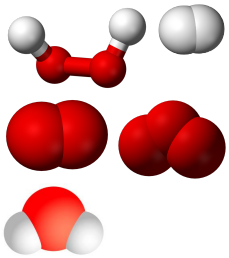
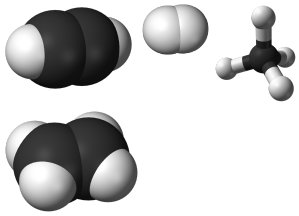
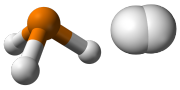
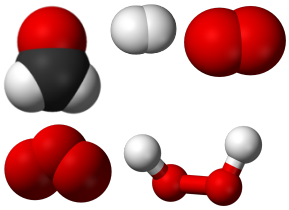
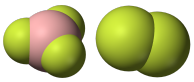
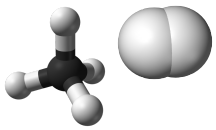
				
Hydrogen/Carbon/Oxygen	H = 1 C = **1** (Never C as connector, O as connector allowed but not molecule) **2** (Never C as connector, H as both connectors allowable but not molecule), **3** (Never C as connector, all connectors as H allowed but not molecule, one connector as O maximum), **4** (Never C as connector, Maximum of one O as connector) O = **1** (H allowed but not molecule), **2** (Never both connectors C)	**Limit 1 carbon**		**CH2O, CO2,CO, CH4, CH3OH, H2, H2O, O2, O3, H2O2**
Hydrogen/Carbon/Fluorine	H = 1 C = 4 (Never C as connector) F = 1	**Limit 1 Carbon, No limit on F or H**		**CH3F CH2F2, CHF3, CF4, H2, F2, CH4, HF**

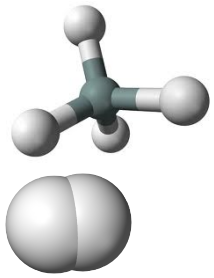
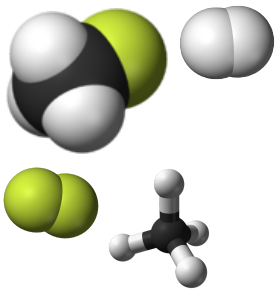
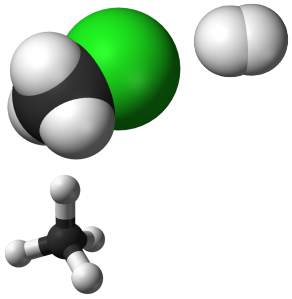
				
Hydrogen/Carbon/Chlorine	H = 1 C = 4 (Never C as connector) Cl = 1	**Limit 1 Carbon, No limit on Cl or H**		**CH3Cl, CH2Cl2, CHCl3, H2, CH4, Cl2, HCl**

Molecules Possible

Name	Possible Scenarios in Kit	Molecule Images	Possible molecules
Hydrogen (H2)	Two atoms together make a hydrogen molecule. Attempts to add a third atom to the hydrogen molecule are all repelled.		**H2**
Oxygen (O2)	Two atoms together make an oxygen molecule. Attempts to add a third atom to the oxygen molecule *result in ozone. Attempts to add a fourth atom to ozone are repelled.*		**O2, O3**

Nitrogen (N2)	Two atoms together make a nitrogen molecule. Attempts to add a third atom to the nitrogen molecule are all repelled.		**N2**
Fluorine (F2)	Two atoms together make a fluorine molecule. Attempts to add a third atom to the fluorine molecule are all repelled.		**F2**
Chlorine (Cl2)	Two atoms together make a chlorine molecule. Attempts to add a third atom to the chlorine molecule are all repelled.		**Cl2**
Carbon Monoxide (CO)	Carbon and Oxygen together from the carbon monoxide molecule. A second oxygen can be added to the opposite side of the carbon, forming CO2. All other additions to CO molecule are repelled.		**CO, O2, O3, CO2**
Nitrogen Monoxide (NO)	Nitrogen and oxygen form NO. Addition of second Oxygen to opposite side of nitrogen results in NO2 molecule.		**NO, N2, NO2, O2, O3**
Water (H2O)			**H2O, H2, O2, O3, H2O2**
Carbon Dioxide (CO2)			**CO2, CO, O2, O3**
Trioxygen or Ozone (O3)			**O3, O2**
Dinitrogen Monoxide (N2O)			**N2O, N2, O2, NO, NO2, O3**
Hydrogen Sulfide (H2S)			**H2S, H2**

Hydrogen Cyanide (HCN)	One carbon, or need to include two carbon molecules.		**HCN, H2, NH3, N2, CH4**
Borane (BH3)			**BH3, H2**
Ammonia (NH3)			**NH3, N2, H2**
Hydrogen Peroxide (H2O2)			**H2O2, H2, O2, O3, H2O**
Acetylene (C2H2)	4 or less hydrogens		**C2H2, H2, CH4, C2H4**
Phosphine (PH3)			**PH3, H2**
Formaldehyde (CH2O)	One carbon only, or need to include two carbon molecules.		**CH2O, H2, O2, O3, H2O2**
Boron trifluoride (BF3)			**BF3, F2**
Methane (CH4)	Limit 1 Carbon		**CH4, H2,**

Silane (SiH4)			**SiH4, H2**
Fluoromethane (CH3F)	Limit 1 Carbon		**CH3F, H2, F2, CH4**
Chloromethane (CH3Cl)			**CH3Cl, H2, CH4, Cl2**

Meeting Notes

April 11, 2001

Discussion between Emil My, Jonathan O, and John B

- We should use the “Pseudo Lewis Dot Structure” for the construction of the molecules in the play area, and then allow them to select a more 3D view in the collection area. JO and JB were wondering if it might confuse middle school students to have different representations, but after discussing it with Emily it was decided that it was okay and perhaps even helpful in starting to understand that all of these representations are inaccurate in some way.
- In the play area, bonded atoms are depicted by having their edges touch. There should be no bond shown, and no overlap for the atoms.
- When the user has completed the molecule collection, they should be shown a dialog that gives them the option to generate a new set.
- The first set of molecules that is show should always be the same so that a teach could talk about the first tab with the students and have everyone be looking at the same thing. However, subsequent generation of molecule collections should be randomized.

March 31st meeting

- what if molecule not intended product
- 2D, pseudo-3D, 3D (show lennard-jones type rep in play area, have option for 2-d or p-3D)
- maybe random appearance of molecule choices
- global options (name/formula?, 2D/p3D)

Prior Art

Molecule Editors

There are a number of "molecule editors" that are available on line. Most of these are significantly more sophisticated than what we are likely to create, but are quite useful as reference points and for ideas. There is a fairly large list of molecule editors that can be found here:

http://en.wikipedia.org/wiki/Molecule_editor

There is one called "Avogadro" that seems quite powerful. It can be seen here:
http://avogadro.openmolecules.net/wiki/Main_Page
There are video clips that show some of what Avogadro can do here:
http://blip.tv/file/1734564

Chemistry File Formats

There are a number of file formats that have been developed to describe molecules. Using one of these may save us a lot of development time, especially if we want to create more sophisticated molecules. Here is a link to a Wikipedia article about some of these formats:

http://en.wikipedia.org/wiki/Chemical_file_format

Discussion

JO/JB questions/comments:

Caption for "Atoms" below the atom bins

EM: I like the idea of labeling atom bins as 'atoms, and the molecule area as 'molecules' to distinguish what's important for the learning goals.

SR: It seems confusing to label the molecule area as "molecules" since you can put one atom in it. Maybe when you construct a molecule it should say molecule as part of the name: "caffeine molecule"

EM: No I am referring to the "collection area" where it lists already constructed molecules

SR: Sounds good.

How can people be able to both move molecules and split molecules apart. Both would use dragging? (Tools?)

SR: Maybe a red 'x' to detach an atom?

EM: Maybe the atom changes color when ‘selected’ and clicking and dragging can ‘select’ multiiple atoms? Maybe that’s too complex?

SR: How does that help split molecules apart?

Do we show both common and scientific names?

SR: I think so, common name should be first

EM: There’s not so many with 2 and 3-atom molecules with common ‘common’ names. I’d rather just use the scientific name if it’s not something a student might use in everyday language.

Should we limit them to try to combine up to 3 atoms at a time so we don’t have conceptual problems about bonding / formation?

SR: I don’t think we should add artificial limitations on this sim, but that leads to a combinational explosion of molecules. So I’m not sure how to productively constrain allowed types.

EM: Once you get to 4-atom molecules, the structure of the molecule becomes more important and you have a huge number of options. I don’t think this is necessary to get at the learning goals for middle school, but for higher level usage, more than 3-atom molecules will be needed.

Do we want the atoms to have the same size? (Somewhat unrealistic?)

EM: yeah, that would be great. Right now the spec only includes four atom types, all from the first two rows of the periodic table, so the size difference is probably reasonable to represent ~ accurately.

What are the incentives or indications to drag atoms / molecules to the left (build molecule area) or the right (collection box).

SR: I was confused about that too, but I think the collection box should be redesigned to be more like a camera/snapshot feature.

JB: Why have a recording feature at all?

JO: maybe so you could have extra atoms to work with, or compare different molecules to each other.

EM: The idea behind this was to add a subtle ‘game factor’. Noah has a game on his phone where he combines earth/wind/fire/water to make different things, and the goal is only to collect a lot of different things. Perhaps they could try to make as many different molecules as possible given the amount of starting materials, or try to use up all the starting atoms without having any leftovers? My original thought is that students would be able to take things in/out of the box to use as materials.

SR: it looks like EM is explaining the box on the right, where it shows what you have attained. We are wondering why to have the box on the left. I do like the “game factor” of highlighting + automatically adding to a list all the different molecules the user made.

Is it a learning goal that two given molecules with the same formula and structure and basically equivalent molecules?

EM: I’m not sure I understand this question...i’ll ask about this during meeting.

What is the importance of the handle on the collection box?

SR: I was confused about that too, but I think the collection box should be redesigned to be more like a camera/snapshot feature.

EM: It was just to give the idea that things were going into and out of the box. It doesn't have to be there.

SR: Based on discussion above, I think molecules should appear in the collection box automatically, without any user interaction.

Could use a right-click menu (or instant popup menu) on bonds or on atoms, to separate it from the rest of the molecule.

What about showing lewis dot diagrams? Or ball and stick model? Some way to show how things can be connected?

EM: Bonding is complex, and is approached (or not approached) in ways that vary significantly from one middle school to the next. Chemistry has an accepted representation ('space filling') that doesn't explicitly represent bonds, so I thought it would be easier to use this representation. We can talk more about this, and I can also ask for outside opinions from MS experts.

Are rules like VSEPR general enough for constructing an arbitrary molecule out of the provided constituents?

EM: Unfortunately, no. The reason there are so many bonding models covered in intro chemistry classes (Lewis Dot, VSEPR, Molecular Orbital Theory and some combinations thereof) is because there is no easy to use general bonding model. Molecular Orbital Theory is the best, but I would definitely not say it's easy to use. In practice, chemists use the simplest bonding model that works for the types of molecules they work with. Even worse, middle school students are often not exposed, or not exposed in a very useful way, to bonding models. For each molecule included in the acceptable set, I'd need to verify the most appropriate structure to represent it (just from an internet search). Otherwise, we might end up with many email corrections from those intimately aware of a more accurate structure.

If we limit the user to creating 3-atom molecules, what do we do when they create things that don't tend to exist very long in nature, like NH2 and CH2? Do these have names? They are close, in these cases, to creating common stable molecules (ammonia and methane in this example) but can't finish it.

- One suggestion was to gray out molecules that wouldn't react and only allow them to create something that exists in nature.

EM: Especially for middle school, I would only want stable molecules to be included. With the amount of information middle schoolers have to work with, understanding an ion/radical, much less molecular lifetimes, is a big challenge.

Comments from SR:

Sim is not yet ready for development, need more pictures of what the molecules should look like.

Get rid of gray rectangle, objects should be interactive immediately after dragging out of buckets

Should decide 3D vs 2D as early on as possible, cannot upgrade from 2D to 3D without throwing away lots of code

-Flex vs Java

-JMol if Java 3D?

EM: In short, I think 2D would be fine for middle school level, but 3D would be better. It would also be interesting to study any differences between students interpretations of the 3D molecules vs 2D. We should

talk more about this topic.

Using a camera metaphor for saving molecule snapshots instead of dragging to a jar.

Drag handle on the name?

Not showing bonds? Isn't that critical to learning about the structure of molecules? Maybe bonding should be in a later tab?

JB: Maybe add an option for “Show bonds on/off” in the first tab?

Why turn H2O x2 into 2H2O? Seems potentially confusing to collapse them in this fashion.

EM: Representing two water molecules as $2H_2O$ is the accepted way to do this by chemists, and is a big challenge for students. It’s the infamous ‘subscript, superscript, coefficient’ battle that all chemistry students must overcome...and all chemistry teachers cry over. This is one of the learning goals of the sim, to help students distinguish between the coefficient and the subscript.

Come up with an internal dsl like: new ThreeAtomMolecule(C, 90.0, N, 180.0, H);
new TwoAtomMolecule(C, N); //etc.
something Emily can verify and contribute to.

Topics for March 9 meeting:
- Labeling of ‘Atoms’ and ‘Molecules’
- Dragging of atoms/molecules
- Common and scientific names
- Limit molecules to 2-3 atoms?
- Show Bonding?
- Role of “collection box”, maybe use ‘snapshot’
- Form unstable molecules/ions/radicals?
- 2D or 3D

Some Notes from 3/9/2011

- Distinguish an atom from a molecule.
- Once you make a CH4, then it should be given a specific solid color, or highlight, and a name
- CH4 behaves differently than just 4 H and a C not bonded together.
- How to go from macroscopic view to microscopic view? Like building a macroscopic fluid from H and O particles.
    - EM: Not addressed directly in this sim, we just focus on the subproblem of molecules being made of atoms
- JB: Should be able to provide common names, right?
    - EM: There aren’t that many molecules with common names, but I think we should provide it if we can.
- SR: What about giving some indication about what atoms can be connected together?
    - EM: Bonding provides many complications that we may want to avoid.
    - SR: What about just showing them as puzzle pieces or equivalent?

    - EM: Maybe we should have the option to show bonds in different representations.
- SR: As you make more and more molecules, it shows “achievement unlocked” and gives the player a title, culminating in “Molecule Monarch”
- EM: Once the user makes enough things, then the buckets refill as a reward
- More Questions:
    - split molecules apart?
        - EM: Probably yes
    - use ball and stick/lewis dot rules for joining atoms?
        - EM: That would probably be sufficient for many cases
    - 2D vs 3D?
        - JB: 2D much faster, but maybe 3D more pedagogical/extensible?
        - EM: Better to have 3d if you can build large molecules.
            - SR: What about flattening the representations?
            - EM: like in Lewis Dot diagrams?
            - JB: is it a learning goal that angles are correct? Will we create misconceptions if we don’t make the angles correct?
            - EM: it would probably be best to keep the angles correct as the user goes
            - SR: Does this mean we wouldn’t want to support methane?
            - EM: well that would require 3d
            - JB: How about first tabs are all in 2d with only up to 3 atoms, but then in later tabs we could show a noninteractive (or just rotatable) 3d representation.
    - Java/Flex/HTML5
    - What is the least constrained case we want to handle?
        - 6 of each atoms

Questions:
What atoms/molecules appropriate for middle school use?
How to scaffold for middle school use?
What level might be appropriate for advanced use (high school/undergraduate)?
Use of Scale for Weight?

- Might help with understanding that matter has weight, even if you can’t feel the weight in your hands. Students understanding of the world around them develops from a concrete understanding of physical objects, including the ability to feel heaviness. Children think that things without weight that can be felt don’t have weight, for example, air. Seems like the use of the scale picture in middle school sims could be important to help address this, though students likely need conceptual reinforcement of what use of the scale means in relation to macroscopic things from the teacher.

Kits:
Kit 1: H2
Kit 2: H20
Kit 3: O2?
Kit 4: CO2
Kit 5: N2

Student Challenges:
Challenges for middle school students:

- Children have difficulty conceptualizing that matter is made up of atoms and that atoms can be bonded together to form molecules. This can be tied in with students having difficulty believing that something exists that has weight too small to measure in their hand.
- Children have difficulty understanding what it means to have a molecule that doesn't change during a phase change, but rearranges in a chemical change. This is also further complicated by ideas of dissociation of ionic compounds.

This seems to me (EM) to be rooted in a lack of development of the ideas of forces as they pertain to chemical systems, and to bonding. Without some kind of framework for intermolecular forces/bonding, it would seem puzzling why sometimes molecules come apart easily, while other times they don't.

Perhaps something like, molecules are bonded together, and some bonds are stronger than other bonds would be helpful.

- Need to be careful in representing very small size. Seems important in some school contexts to be able to articulate that atoms are too small to see with magnifying glass or light microscope. Don't want to represent something meaning 'very small' but give the impression that might be seen through a microscope.

References:

- Harrison, A.G. & Treagust, D.F. (2002). The particulate nature of matter: Challenges in understanding the submicroscopic world. In J.K.Gilbert, O.D.Jong, D.F.Treagust, & J.H.van Driel (Eds.), Chemical education: Toward research-based practice (pp. 189–212). Dordrecht, The Netherlands: Kluwer.

- Liu, X and Lesniak, K. *Journal of Research in Science Teaching*. Progression in children's understanding of the matter concept from elementary to high school. (43) 3, 320-347 (2006)

Garnett and Hackling (1995) and Snir, Smith, and Raz (2003) concluded that students' inability to visualize the particulate submicroscopic nature of matter represents a major area of difficulty in developing a sound conceptual understanding of chemistry. A 3-year longitudinal study of 11- to 14-year-olds' conceptions of matter by Johnson (1998) found that students' conceptions of particulate nature of matter may progress through four stages: (a) No particulate notion exists, (b) particles exist separately from substances, (c) macroscopic particles make up substances, and (e) microscopic particles make up substances.

- Wiser, M and Smith C.L.The International Handbook of Conceptual Change. Edited by Stella Vosniadou. (2008)

Beautiful description of the evolution of children's understanding of matter from infant up through middle school. Great argument for starting the introduction of "matter is made up of atoms" very early, and to take the approach of starting from children's natural thought tendencies and building up. Also describes a non-useful model that students can development (atoms are in matter) as compared to a useful model (macro-particle, in which students recognize that matter is consists of atoms, but still ascribes macroscopic properties to individual atoms), which seems to bridge the macro-continuous with the micro-particle views.

Interview Feedback

MS4M4
4/18/11
Version: 0.00.04
Age: 9
Grade: 4th
School: Mesa Elementary
Sim Use: Interviewed once before
Also interviewed for SOM

Tab 1
- why are their two “make a molecule” tabs
- makes hydrogen immediately, tries to add oxygen, doesn’t go
- notices that the toolbars are different in the two tabs
- makes oxygen, tries to put together, won’t go.

2nd tab
-makes hydrogen peroxide, says the name
- tries 3rd tab, i explain that this tab doesn’t work, goes back to 2nd tab
- “how does it work” if the only thing you have is this [first kit] then you put them all together and it tells you what it is?”
- finds next kit button while talking
- makes carbon monoxide then carbon dioxide
- describes how di means 2 and mono means 1
- Makes nitrogen, splits apart, tries to add nitrogen to CO_2, won’t go
- splits apart all molecules, makes NO and NO_2 (i think he predicted this from the CO and CO_2 cases previously)
- Finds third kit in 2nd tab “there’s alot...there’s 7 hydrogens”
- starts adding H’s to CO, tries to add N, makes N with 2H’s from the repulsions making atoms bump into each other.
-Plays around, says ‘wait’ seems to be thinking, maybe looking for patterns
-I ask what he thinks about atoms that stick together but don’t have a name
- “because this one, and this one [clicking the x on connected atoms that are unnamed] aren’t actually atoms...i mean molecules... that have been made...that exist”
- plays around some more
- tells me what molecules he’s made, and that he can put together two carbons
-switches to fourth kit, makes hydrogen, HF, HCl, fluoromethane “sounds interesting”, thinks that if he takes off the F, he’ll get methane, but sees that this is not correct when no name appears.
-goes to next kit, then moves back to first kit
-notices the collection box again, and that he needs to make $2CO_2$,

- tries to make this by adding O to the O side of CO, doesn't go.
- Makes oxygen and puts it into box, reads out loud "you have one O2"
-goes through and starts making molecules for the collection boxes, switches through kits easily looking for what he needs
- can't find what he needs for 2H3N, breaks apart molecules by putting back into kit
- realizes that he has extra N in one kit, and extra H in another, but can't put them together.
-I tell him that it's a problem with the sim, that he doesn't have everything he needs, so it's ok to stop looking
- he plays around some more
- wants to know if he can take things out (still trying to find what he needs)
- i suggest that he might be able to find everything he needs for the first tab
1st tab
- goes through easily and fills up the collection boxes
- tries to make H20 by making hydrogen and adding oxygen, realizes he needs to split up the hydrogens and add them to the oxygen
- I ask why the molecules look different in the boxes
- he says it's probably because something with the computer makes it so it can only go in that way, says he's probably wrong though.
- he recognizes that the diatomics don't really change, but that water did (bent instead of linear)
- compares the case with water linear in play area with water where the hydrogens are on bottom and side, says they're both the same.
- sim is 'interesting, and actually has something you need to do
- "they should fix having everything you need and the third tab"
- I asked him what he learned, he lists off molecules and starts building some to show me
- Reiterates how it should be fixed so that he could make all the molecules
- I ask how he knew what the coefficient was, he describes to me what the subscripts "the opposite of exponent" means and that the number in front means how many of them you need
- says if i tell him when everything is fixed "i will probably play this"

US1F
4/22/11
Version: 0.00.8
Year: Junior
Major: MCDB, may change to Psychology
Prior Science Coursework: No Physics, Gen Chem I, II
PhET Use: About 3 sims in previous courses
10 Minutes Total

Tab 1
"Sweet, I love playing building games"
Puts O-H together, sees x "does that mean I'm wrong?"

Adds another H, says “what’s that little x?”
Finds 3-d button, clicks a couple of times, box pops up “cool, it’s like water”
***Makes NO2 from Kit #3, no name appears
Clicks x, seperates atoms, makes water again
Sees blinking blue outline, puts water inside collection box
Clicks reset kit
Tries to make oxygen, “I can’t make it...because I don’t have another one [oxygen]”
Finds kit arrow, “ohhh, I get it”
Makes another water, makes oxygen
Asks if this is for intro to chem.
Tries to place atoms in correct geometry, for example, hydrogens of water in bent position, doesn’t seem bothered they click into lewis-dot structure arrangement
Continues to fill up collection box as she goes through the kits, making other molecules along the way
Selects to have new collection boxes “yay!”

Wonders if she can do it wrong...tries to add a hydrogen to a hydrogen in Ammonia, hydrogen is repulsive. “cool”
Tries to make H2O2, doesn’t know structure. Makes water tries to add Oxygen to it, won’t go. Takes it apart, makes O-H and O-H and puts them together.
Fills up second set of collection boxes

3rd Tab
I remind her that she can stop whenever (this is her third sim for the hour)
She wants to play with 3rd tab before stopping
Tries to make something that won’t go, wants two oxygens on a carbon, figures it out.
**Can’t add third carbon to C-C-O2 chain...
Likes that it tells you what you make
Says that it must mean it’s not anything if no name shows

General Notes:
-Sim didn’t recognize NO2 as molecule in first tab
-I’m slightly concerned about the limitations of the last tab, will need to make clear about that in Teachers Tips.

MS2M6
4/22/11
Age: 12
School: Southern Hills Middle School
Sim Use: Used many PhET sims previously, Teacher is Kathy Briggs
Also interviewed on SOM and EFH

Tab 1
Makes water

Finds 3D easily, clicks many times before window opens

Tab2
Makes H2O2, looks in 3D
Doesn't notice the kit change

Tab 3
Uses x button easily
Moves object in 3D, changes between representations
Finds kit arrow

MS10F8
4/27/11
BAM
Version: 0.00.10
Grade: 8
School: Summit MS
PhET Use: Used 1-2 in class before

Tab 1
"oohh wonderful"
Pulls out O, attaches H, sees x "not a molecule...means something else"
Adds second H, sees arrow, puts in collection box.
"Is this the law of multiple proportions illustrated?"
Makes H2O2, tries to put in boxes, won't go
"Hmm, it's fun, hydrogen peroxide is interesting"
Kit 3
Starts trying to put them all together, "I have no idea what this is going to be"
"I like that they are big and labeled"
"This will only work in a certain way..."
Makes NO, splits molecules, makes O2, puts in collection box
Apparently "C, N and N doesn't work"
Makes NO and NO2 "that one at least is the law of multiple proportions"
Uses reset kit
Makes H2, makes O2, "ahh, I get it"
Flips through kits to fill collection box

Sees that collection box refills, gets really excited “this is awesome!”
Makes water, ozone,
“I kind of get one of the messages of this, most of the things we encounter in daily life aren’t just one atom acting alone, there are all these atoms together”
Makes phosphene “I wonder what kind of molecule this is?” clicks around, finds “+” sign
Opens 3D “ooh, a 3D perspective of phosphene, that’s awesome” puts in collection box.
“haha, you are mine!”
Likes colors of atoms
Fills up collection box again “ohh, are there even more molecules?!”
Makes methane, “this is interesting molecule, I think I like it...on the other hand it is destroying the world”
Makes acetylene
Describes structures in collection box, some are ‘tripods’
Uses formula to determine structure, rearranges when initial guess doesn’t work
“the chemical formulas suddenly make sense, they’re in some kind of order”
“Scientists don’t like coincidence, well, they’re great fans of it as long as turns out its something that can be measured and quantified”
“Fluorine! Not flour-ine, which is how people keep spelling it in my class”
Tries putting molecules together in order, as in CH3F means H bonded to C and F bonded to H, doesn’t work, figures it out
Comments again how things you interact with everyday aren’t just single atoms
Tries pronouncing trifluroborane, laughs.
“that’s why it’s called trifluro...it has three fluorines!
Sings “I get chemical formulas”

Tab 2
Reads collection box...”goal: 2O2, you have none...”
Puts individual in box, pause...”ahh.” notices that it counts the molecules
Adds in multiples into box.
Gets to the last one, with no O and Carbons left “I loose”
Figures out that “reset kit” only resets that specific kit, figures out how to fill up the rest

Tab 3
“Looks interesting...what am I supposed to do with these, just play around?”

Talks about how some want to bond with each other, while others do not. “I wonder if carbon is just evil?”
Makes hydrazine, says it’s N2H4

What do you think about this one?
“it’s really fun. I like putting things together and seeing what they make.”
‘It’s very interesting to be able to see it, even if it’s just virtual”
Likes trying to pronounce names
“I wonder what nitrosyl hydride looks like...oh, I can use 3D”
recognizes that there is a structural difference between what the molecules look like in play area and what they really look like
Tries to use up all atoms in Kit #1, has some hydrogens left over “I loose”.

K1M8 (not sure how to label)

04/29/11 v 0.00.12
Male, 14 years old, in 8th grade at Centennial
Likes US history, learning about Einstein in science
No PhET sim use

1st tab:
Makes H2O, drags around, clicks on blue arrow, resets kit
Next kit, makes O2, resets, makes H2, next kit
Makes COO (not CO2), resets, makes N2, resets
Says easy, wonders if more to do
Tries to use all atoms, but can’t; resets, tries again, still can’t, breaks apart
Says he feels like he’s just messing around
Already knows combine in chemical rxns, create new things using elements on PT
Ask him about flash: says it means he’s completed the task; says you clear (reset) and make another
Says the red button splits it
Ask him about other button: clicks, says did not expect that, did not try to move
Clicks ball-and-stick, says did in 6th grade, but not on computer; closes window
Ask him to make water, tell him to drag over (after 7 mins)
Says maybe it should go over automatically after you make it
Makes COO, tries to put in, did not go; break apart, gets it
Fills up, clicks new molecules; makes H2, says oh, the arrow points to it
Makes CNH (not HCN), tries to put in, breaks apart, gets it
Fills up, gets new molecules

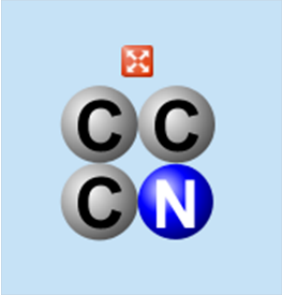
Makes SOO (not SO2), tries to put in; uses arrow to break one bond (accident?)
Says maybe if put in extra ones that you don't need, would be more difficult
Makes HCOH (not CH2O), tries multiple times, goes to next kit; comes back, gets it
Fills up, gets new molecules, etc.
Spent 14 mins on 1st tab

2nd tab:
Ask him if noticed the tabs
Figures out that he has to reset kit to fill box
Says this tab more difficult; you need to go back and reset kit
Says maybe if spread out over kits, would be more difficult, rather than one kit for each box
Says if you had to hunt, rather than disappear when switch kits
Wants name of molecule in collection box; did not notice name over molecule
Gets confused by 2H2S at first
Ask him if fun: says good learning device for 6th grade; use PT in 8th grade
Spent 12 mins on 2nd tab

3rd tab:
(Note: can make squares; see image)
Says maybe if put # of protons down here, you could tell if you made the max amount (of bonds)
Says he's trying to figure out how many protons Cl has; knows H has one
Adds H's to atoms: says max # of protons is 8; no, electrons (corrects himself)
Says H has 1 proton & 1 electron; C needs electrons, you can add H to see how many they need
Confused why some have name & some don't: CH4 is methane, CH2 has no name
Says maybe say unknown name, or not real molecule, or complex name
Tries to "max out" molecules (see how big you can make it)
Starts putting H in center of atom instead of side
Says he has one H atom left; trying to use all atoms up
Ask him if learned: says easier than what he used in 6th grade because you get an unlimited amount of pieces on the computer
Spent 13 mins on 3rd tab

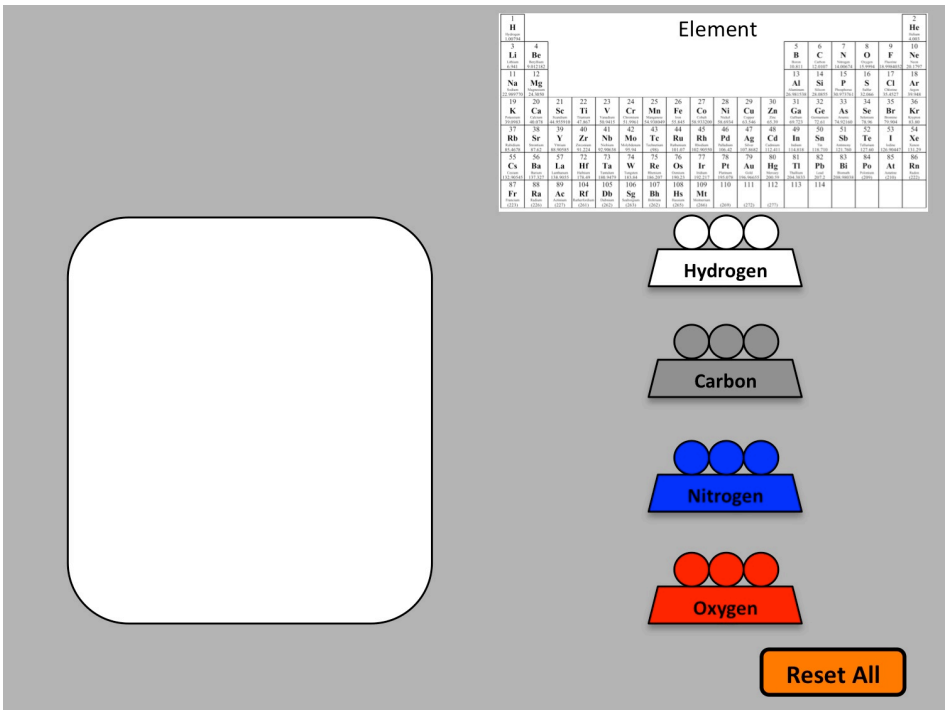
Notes:
1st tab:
Had to tell him to drag molecules into collection area
Only opened 3D once when prompted, then never again
Did not notice the name over the molecule in play area
2nd tab:
Had to prompt him to open next tab
Figured out that he had to reset kit to fill collection
3rd tab:
Added H to atoms to figure out the max # of bonds (but did not say "bonds")
Started to put H in center of atom instead of side
Confused why some have names & some don't

Tried to make big molecules, then tried to use all atoms up
Fix: you can make squares (see image)



OLD

1st Gen First Tab



Mock-up Design Elements:

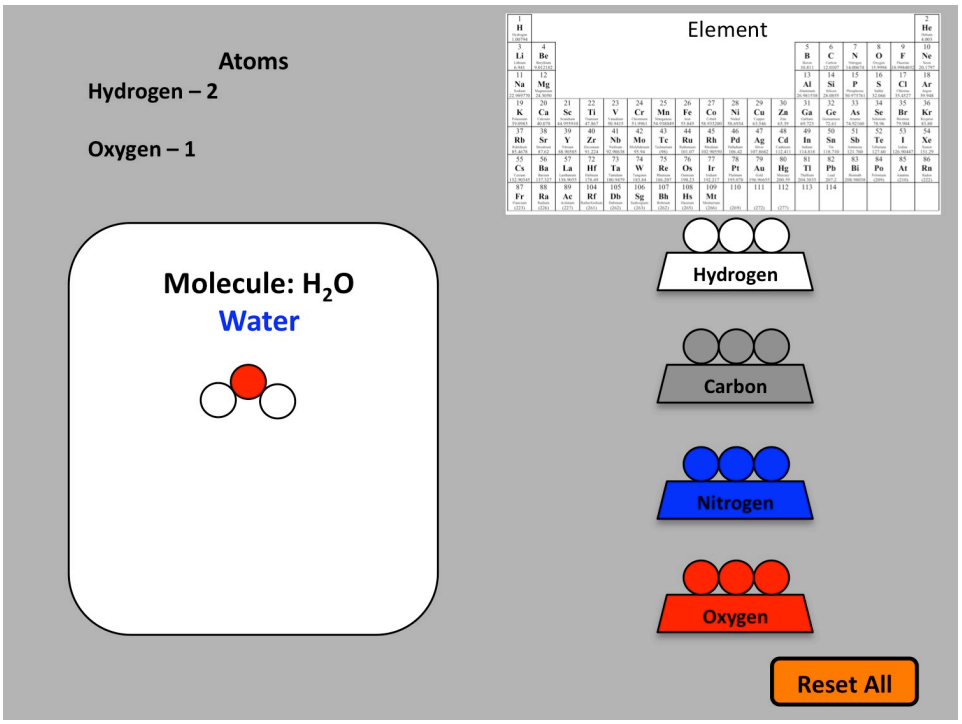
Note: Atom colors match those found in Balancing Chemical Equations

Periodic Table: Has the first three rows as buttons (or the elements available for building as buttons)

Atom Buckets: Upon selecting an element, the ‘buckets’ show up with the different options of other elements to combine with to make a molecule. I’m showing four here, but maybe could be as large as eight (two columns of four buckets).

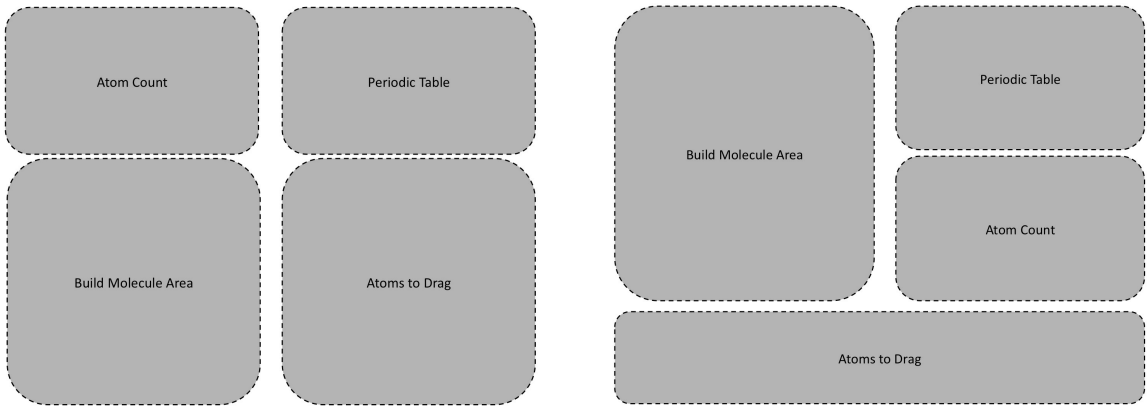
Molecule Building Area: This is where you’ll drag the atoms from the buckets to form the molecule.

Atom List: As you build a molecule, a list of what atoms you’ve used will appear above the Molecule Building Area.



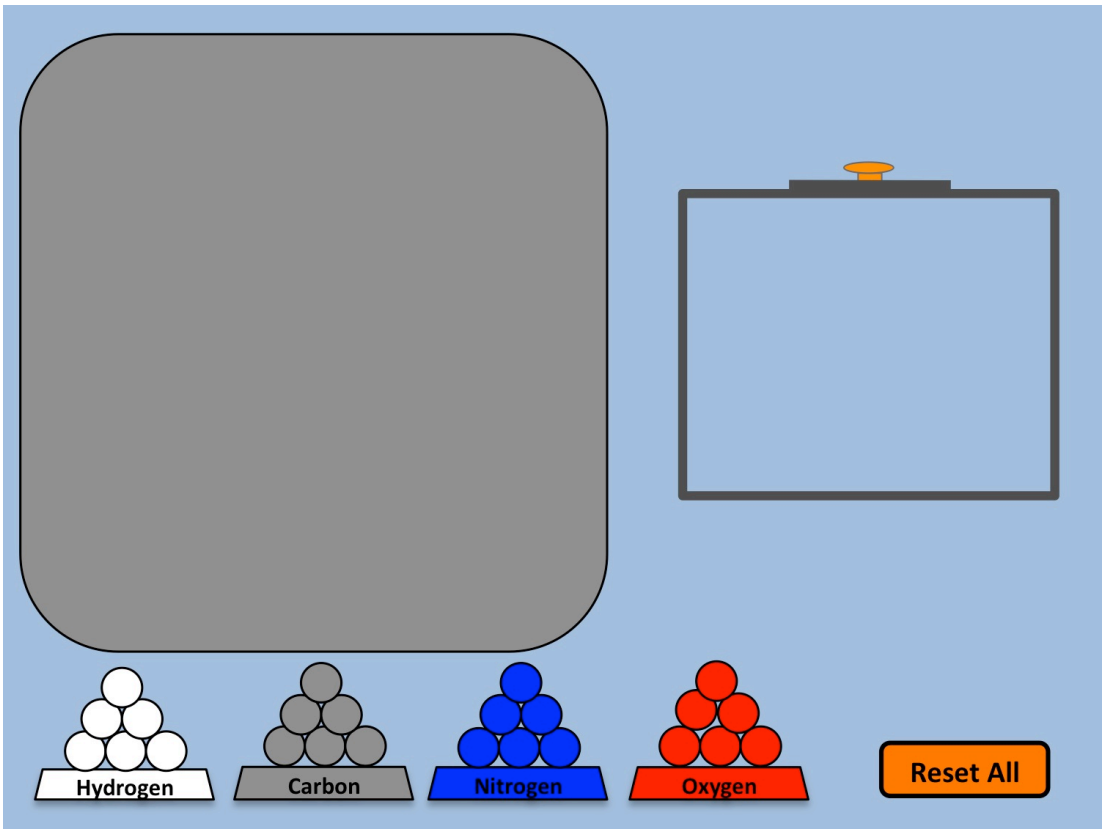
Different Layout Possibilities

First one is what is shown in mock-up above, second is a different option



or

2nd Gen



Mock-up Design Elements:

Build Molecule Area: Students can drag atoms from the atom stacks and play with rearranging them. Many atoms can be in this space, but once atoms that together form a molecule come close, they must change into a 'final' form to signify that a molecule has been made.

Molecule Name: The name of the molecule must appear near the newly formed molecule. Students then have the option to move this new molecule into the collection box or not. If they don't move to the collection box, the name will disappear and the constituent atoms can be used to make some other molecule.

Collection Box: If the molecule is moved into the collection box, then the name of the molecule appears in the collection box near (above or below?) the molecule. If two of the same type of molecule are added to the box, only one molecule is shown, but the label changes (example: From "H_2O" to "2 H_2O").

Molecules can be removed from the box and placed back into the build molecule area.

Scaffolding for Middle School:

Changeable Components:

- How many atoms/molecules available: a lot or a little
- Adjusting the number of atoms in the buckets: to be exactly what is needed, or just keeping the same amount regardless of allowable possibilities for molecules
- Atom Count region: Show or not

Simplest
Option 1:
- Only a few atoms to choose from, and a small set of molecules that can be made.
- Once an atom is placed in the Molecule Building Area, all the available buckets become filled with only the appropriate number of atoms to make the possible molecules. (this might minimize time spent randomly trying to add atoms to the Molecule Building Area.)

Option 2:
Same as Option 1 +
-No atom counter area shown (this might be good for a teacher who only wants to qualitatively introduce the idea of molecules are made from atoms)

Option 3:
-Same as Option 1 or 2, but don't change the number of atoms in the buckets to fit the number needed to make a molecule. This would increase the difficulty of finding all possible molecules.

Most Difficult
Option 4:
- Maximum number of possible atoms/molecules
- No constraint on the amount of atoms in buckets, students will have to figure out what works

Online Resources
Possible list of atoms to choose from (from middle school resources):
H, C, N, O, Cl, S, Na, Mg
Possible Molecules (Seen in middle school resources):
Water- H20
Methane- CH4
Ammonia- NH3
?Nitrogen- N2
Salt- NaCl
?Chlorine-Cl2
Ozone-O3
Hydrochloric Acid- HCl
Sulphur Dioxide-SO2
Oxygen-O2
Sodium Hydroxide- NaOH