Thoughts on Visualizing Chemistry

multiple representations to assist understanding

Lauren McCafferty
Thoughts on Visualizing Chemistry: multiple representations to assist understanding

Thesis presented by Lauren McCaffery to The Department of Art + Design as partial fulfillment of the requirements for the degree of Master of Fine Arts in Information Design and Visualization at Northeastern University, Boston, MA, May 2015.
Organic chemistry is a fundamental course for any student who wants to pursue a future in medicine or the science field. How do we comprehend a topic so abstract yet so critical? How can different methods of visualizing the same chemical reactions be a system to aid understanding?

Chemistry cannot be seen. We can see evidence of it taking place, but the actual renderings occurring in the atomic scale are invisible to our eye. There exists a broken visual circuit between the flat two-dimensional line drawings of molecules and the three-dimensional dynamic molecules that they represent. This thesis is an exploration of visual notation methods used to illustrate chemical reactions, the translation of the reactions into choreographed dance pieces, and how understanding is facilitated through parallel representations.

We coexist on many micro — and macro — scales simultaneously. The same principles apply to the world of chemistry. There exist unique tensions and balances that are currently lost in the visual methods used to depict these delicate structures. Translating the atomic scale reactions of chemistry into multiple representations can allow students to choose their own methods of learning, and thus perpetuate understanding of the subject as a whole.
I would like to first and foremost thank all the faculty members of the Information Design and Data Visualization MFA program here at Northeastern University. You have cultivated a space for learning and designing and a program that I am sure will only become better with age, and I am honored to be part of the first class.

To my classmates — we have paved the way. I would not have been successful these past two years without the ongoing support I have felt from all of you. Our long nights and hard work has paid off.

acknowledgments

To Thomas Gilbert, for understanding my vision and assisting me to make this project chemically sound.

To Stephanie Trowbridge — I have learned so much from working for you these past two years. Thank you for giving me an opportunity to discover my creative freedom within Academic Technology Services while also helping me cultivate a new knowledgebase between teaching and technology.

To those who helped create the performance piece to my project: Laura Stoffko, Janna Mino, Julie Smilak, Leanna Wanta, Victoria Busbee, Christine Rutkowski, Nicole Evans, Melissa Corlett, Bryan Threlfall and Chelsie Richter. Thank you for your late-night commitments to help me bring this project to life. Also to Poppy Dinse for your constant support through my pursuits in life and for reminding me that I always have a second home and family in dance.

Finally, to my advisor Douglass Scott who has helped me realize my vision for this project. And all in all, for your guidance I have not only developed as a designer — that I am forever changing your knowledge and wisdom with me over the past two years. I could not have imagined this program or this thesis project without you.
H represents one atom of hydrogen. One carbon atom, one oxygen atom, and three hydrogen atoms are connected by bonds, making up a molecule. Each line represents a bond, and a bond is made up of two electrons. Two electrons that are not bound to another atom are called lone pairs. The C, H, and O are all atoms, but they are different elements. All of these atoms and bonds together make up a single molecule.

glossary

reaction  a process in which the structure of atoms or molecules that make up a substance are changed

molecule  the smallest unit into which a substance can be divided without chemical change, usually a group of two or more atoms

atom  the basic unit of a chemical element

electron  the part of an atom with a negative electrical charge, which moves around the atom's nucleus

element  a substance that cannot be broken down into any simpler chemical substances

bond  an electrical force that holds atoms together to form a molecule

element  a substance that cannot be broken down into any simpler chemical substances

atom  the basic unit of a chemical element

electron  the part of an atom with a negative electrical charge, which moves around the atom's nucleus

bond  an electrical force that holds atoms together to form a molecule

atom  the basic unit of a chemical element

electron  the part of an atom with a negative electrical charge, which moves around the atom's nucleus

bond  an electrical force that holds atoms together to form a molecule
Signing up to take organic chemistry in college, you feel like you've failed before you begin. The first day seems okay, but soon enough the lectures move at an unattainable speed where you continuously diagram for the fifty minute class, you stop writing mid-sentence of the last paragraph because you're behind and you're professor has already moved into the next reaction. Recitation classes are supposed to give the small classroom-like feel, but really only focus on trying not to fail the quiz each week. "Studying" becomes endless cycles of practicing problems and rereading notes trying maybe if you draw out the reaction one more time, you'll be able to draw Step 4 of 10 when the exam is in front of you. The goal shifts from learning the material to just scoring something, trying to calculate the curve, and crossing your fingers that more people do worse than you.

**introduction**
Most of the real diversity in evolution has been small-scale. We large things are just flukes—an interesting side branch.

Of the twenty-three main divisions of life, only three—plants, animals and fungi—are large enough to be seen by the human eye, and even they contain species that are microscopic...The world belongs to the very small—and it has for a very long time.

Bill Bryson, *A Short History of Nearly Everything*
When beginning to think about investigating the space between visual representation and the subject of chemistry, I recorded the ten values that I thought most important that my final design have. Throughout this entire process I have had a strong desire to create a cohesive system of representation where there are multiple ways to interact with the subject material. I wrote this list at the very beginning of this thesis, and throughout this process, it has become a list of checks and balances to refer back to as a way to stay true to my final design.

1. The design is system-based.
2. The design uses abstract representation.
3. The design allows for transformational model changes.
4. The design provides an interactive experience.
5. The design is easily understood on a scale to understand.
6. The design allows the dynamics to be preserved.
7. The design is engaging to the user.
8. The design can work in conjunction with different physical essays.
9. The design is an aid and a tester.
10. Students would choose to use that material. 
Chemistry is present every second of every day. It is the mechanisms by which our body functions, the way in which photosynthesis take place, and chemistry is behind all the materials we use in life — from steel to plastic. Everything we see and touch has been manipulated by chemistry at some point. Furthermore, the most interesting part about chemistry is that we actually cannot see it taking place.

All of these dynamic interactions, exchanges, and transformations exist on an atomic level that is invisible to our naked eye. We cannot see a water molecule, but we know that at some point, there are enough water molecules to make the sea. To the right is a comparison to help rationalize the actual size of a water molecule.

- The approximate number of grains of sand on planet Earth: 7.5 quintillion
- The number of stars ever recorded in the universe: 70 sextillion
- The number of water molecules in ten drops of water: 70 sextillion

**Chemical notations**

7.5 quintillion or $7.5 \times 10^{18}$

70 sextillion or $7.0 \times 10^{22}$

70 sextillion or $7.0 \times 10^{22}$
Since the end of the nineteenth century, chemical molecules have been represented graphically as a way to have a better understanding of the structures and reactions taking place on the atomic scale. As understanding about the subject of chemistry grows, the models become more complex and informative. The methods of representation have also grown parallel to technology.

There are many different ways to draw the same molecule, and each method offers different information within its representation. Also there are different ways of visualizing molecules as an actual form. There are different three-dimensional forms that the atoms and molecules can take on as a way to give a better overall understanding of their shape in space.
Although they all appear very different, each of these diagrams represent the same molecule, ethanol.
The bond-line form of notation is one of the most explicit notation styles because it shows not only all the atoms present in the molecule, but also the orientation and type of bond between each pair of atoms. This style of notation is easy to draw and does not reflect any special orientation or three-dimensionality. Bond-line structures show an unobstructed view of information, but this form works best when the molecule is smaller, as the chemical structure could get very crowded as the molecules grow more complex.

Lewis dot structures follow the same methodologies as the bond-line formation but also incorporates one additional level of detail — it shows the two electrons between the atoms. The electrons are a more true representation than the single line bond, as every bond is a pair of electrons whose force is holding the atoms together. The lewis dot structures also give more detail to the configuration of the molecule when less than four bonds are present.

The condensed form lists the molecule’s atoms from left to right. This particular style is most beneficial in terms of easily using a word processor to depict the structure. Also, the numbers of each atom are easily counted since there are subscripts for some of the atoms. This structure does require some understanding of how molecules connect since this style does not explicitly show that all four C’s are attached in a row, and the H’s connect to the C that they follow. The condensed form also works best when molecules are linear.

The skeletal form molecules are represented by a zig-zag line denoting a chain of carbon atoms where each “point” is an atom, and the line in between represents the bond between the two atoms. This form also calls for an inference for the viewer to know that there are multiple carbon atoms in a row. Once it is understood that the form represents carbon atoms and hydrogen, it can be combined with the bond-line notation to show other atoms.

The wedge and dash notation is a way to show three-dimensionality on the flat plane of the page. It follows the same system of the bond-line form, but includes new notations for the “dashes.” The wedge notation indicates that the bond and atom are going into the page, and the dashed line represents atoms coming out of the page. The solid lines, as seen before, represent atoms parallel to the plane of the page. This notation style is easy to draw, and adds another level of detail that gives the molecule a special organization on the page.
Newman projection

The Newman projection was invented by Melvin Spencer Newman in the 1950’s while he was a professor and research chemist at The Ohio State University. It was the first attempt to show a three-dimensional molecule in a two-dimensional space. While the molecule is the same as the bond-line form, it is rotated from being flat on the page to viewing the molecule into the page from one carbon to the next carbon. This projection has been almost completely replaced by the wedge and dash notation.

Fischer projection

Similar to the bond-line notation is the Fischer Projection. It is a projection style that takes the wedge and dash notation, and then translates it into a flat projection. Looking at a Fischer projection, the atoms on the right and left of the center are depicted as wedges, and the atoms on the top and bottom are the equivalent of dashes.

space-filling

The space-filling model is another example of a 3D representation of how the atoms arrange themselves. Color and size are used to show representation to different bonds between different atoms. The space-filling model is similar to circles to represent the atoms, but it has removed the solid representation of each bond and shows the molecules nesting into one another.
Edward Tufte’s visual experimentation with translating square dancing image-based notation into symbol-based notation.
Painting by Sarah Combs, a progression of a dancer through time and space.

Notating dance choreography has been considered one of the more complex systems to represent on a two-dimensional plane. Dance occurs over time, with movement, and through space, and visualizing these characteristics can be quite challenging. There have been several attempts to create notation systems. Both of the methods seen here articulately express on paper and the screen what, where, and how the dancer is moving throughout the piece.

This chapter parallels the two major types of chemistry notations: hand-drawn techniques such as the bond-line and then digitally created notations like the ball-and-stick. One of the choreography notation types was created to be hand-drawn while the other notation style is exclusively digital.
Movement-thinking could be considered as a gathering of impressions of happenings in one's own mind, for which nomenclature is lacking. This thinking does not, as thinking in words does, serve orientation in the external world, but rather it perfects man's orientation in his inner world in which impulses continually surge and seek an outlet in doing, acting and dancing.
Labanotation is a system of hand-drawn dance notations, and the creator Rudolf Laban first published the method in the 1920s. The method is based on a system of drawn staffs (similar to music) that are filled with different geometric shapes that represent different parts of the body, and precisely how that body part moves during those exact counts of the music. The notation also visualizes how long each movement takes, as well as where the dancer’s body weight should be placed during the movement. In combination with types of movement such as jumps and turns, the Labanotation is considered the most detailed manner to archive a dance performance through notation. Understanding these diagrams is the key to exact replication of a performance and a way to visualize the movement of a dancer over time, in space, and throughout interactions with other dancers.

Looking at the different parts of the notation method, it is clear that the language is similar to any other language, and it takes time and practice to understand the meaning behind the symbols.

A: Line at the start of the staff
B: Starting Position
C: Start of movement
D: Beats of the music
E: Divides music bars
F: End of movement
G: Large numbers for the bar
H: Small numbers for the beat

The music staff runs vertically from bottom to top. The staff has many different components seen in this labeled diagram.
The music staff is also divided into five vertical columns that correspond to the different areas of the body:

- L: Left side
- C: Center line
- R: Right side
- 1: Body support column
- 2: Leg gesture column
- 3: Body column
- 4: Arm column
- 5: Head column

The notations for each part of the body are drawn in their corresponding column to refer to which part is currently in motion.

The actual movement of the dancer's body is visualized using this system of notations:

- P: Place
- F: Forward
- R: Right
- B: Back
- L: Left

The 45 degree intermediate positions are also seen here.

The three levels of shading are used to represent the spectrum of whether the dancer is standing tall and vertical (U) or moving low to the ground (D).

The pins section of the notation follows the same directions as the movement notation just described. The difference is that the pins are specific notations to describe how the head is positioned and moving during that specific bar of movement.

To the left are examples of arm and leg movement notations which correspond to their corresponding location and height of the specific limbs.
Labanotation goes into even more detail to describe different angles beyond 45 degrees of each body limb. There also is a different symbol for all the joints in the body as well as the different parts of the feet.

The detail-oriented nature of this notation method leaves nothing to imagination when thinking about the movements. Each movement can be replicated completely which was the goal of notating dance with Labanotation.

Static representations of moving bodies is a challenge as flat drawn surfaces can only easily translated into dynamic three-dimensional forms. This is a parallel to chemistry notation as the same challenges are presented when trying to notate dance or a chemical reaction.

Looking at these examples of how other professionals have tackled the issue serves as inspiration as different means of understanding this visualization problem.
Two images from the interactive visualization platform

synchronous objects
Synchronous Objects is an investigation of “the interlocking systems of organization” in the choreography of William Forsythe’s One Flat Thing, reproduced (2000). The choreography is translated into a notation system that converts the movements into data points. These data points are then used as the foundation to re-visualize the movements as objects. This notation method is a combination of many different components that all overlay into one digital interface. The video-screen has three different camera views of the dancers performing the choreography. They can be viewed from the front, from the top, or from within. Each perspective gives the viewer different kinds of information, and a different way to experience the movement. The interface also gives the viewer the choice to experience a picture-in-picture view to show two perspectives of the dance simultaneously and their power to overlap different levels of information.

Visual annotations cue the movements of one dancer and signals other movements to begin. Each dancer has a color that corresponds to their outfit color. Lastly, the interface allows the user to pick between silence, a single, or multiple levels of audio information. Ambient noise, a musical score, Forsythe’s verbal cues, and his commentary are all layers that can be added to enhance the audio complexity of the piece.

The bottom half of the screen is devoted to rating the data points of the movements in real-time. Each dancer has a color that corresponds to their outfit color. Lastly, the interface allows the user to pick between silence, a single, or multiple levels of audio information. Ambient noise, a musical score, Forsythe’s verbal cues, and his commentary are all layers that can be added to enhance the audio complexity of the piece.
MovementDensity tracks the dancers’ movements within the performance space. The areas with the most traffic correlate to the areas with the highest peaks. These data points have been manipulated into many different dynamic objects that algorithmically translate the dance data into different representation forms. Each object is subjected to one feature of the dance such as a density map of the stage which showed the frequency of the location of their movements, and then visualized the information as heat map videos. Other visualizations include 3D forms visualizing the dancer’s body movements, event lines based on the cue data, statistical forms generated through video to show movement, and data visualizations that related the dancer’s current coordinates on the stage with their cue data.

The data points collected from the bottom of the Synchronous Objects interactive platform are converted into different visual representations that highlight different parts of the data set. NoiseVoid shows the amplified noise in the source video, as the dancers perform the piece, the visual noise is carved away in those areas. 3DalignmentForms translates the dancer’s bodies into three-dimensional forms whose arc-like movement is the mirror of the way their arms and legs move within the dance.
Movement Volume translates the dancers themselves as well as the paths they take into abstracted dynamic three-dimensional forms that move through space.

Center Sketch marks every dancer’s placement as a dot, the colors start as red and as the dance progresses, each dancer’s location changes to green as they move through the piece.

Creating a new chemistry notation method
The beginning of my investigation began from the idea that in all representations, whether two — or three — dimensional, the molecules had no orientation with space. The molecule merely floats on the page. I began by building molecules out of foam balls and toothpicks and then photographing them with a hard light. Then I took these images and combined them in Photoshop with flat shapes.

Creating these molecules through this process allowed me to think of them within different physical planes, and it also further provoked my interest in exploring these forms, and thinking critically about how they connect as well as how to show dynamics within a still image.

These initial sketches were my breakthrough moment when thinking about simple shapes other than circles that could be used to represent molecules. I was exploring points of attachment between shapes as bonds rather than representing bonds as distinct lines. I initially was working with triangles, but then I realized that four was the best number since elements cannot stably attach to more than four other atoms at one time. From that point on, I decided to pursue a notation based on square forms.

The following progression of diagrams were created in series where visualizing the Glucose Fermentation reaction was the goal.

Using the bond-line notation form, this is the reaction of glucose fermentation.

I explored notating only the first few steps visually.
Also important to this notation method was the static depiction of movement. As stated before, choreography and chemistry exist as two unique examples where dynamic three-dimensional forms are often seen as flat images on a page.

Simultaneous to this chemistry notation investigation was the exploration of how different artists and designers found solutions to portraying movement within a static surface in the first two examples. The second two examples are photographers attempt of showing movement of real life objects in a single still frame.

Giacomo Balla’s Dog on a Leash embodies the sense of movement through repetition and slight transparency. The dog’s torso and head remain relatively stationary, while its feet, tail and leash are painted multiple times. Also, the slight fade towards the ends of the paws gives a sense of very quick movements that cannot be seen in detail, only the suggestion that the paws were briefly in that position.

Nude Descending Stairs by Marcel Duchamp is a cubist-style painting where the same figure is painted multiple times, where each new figure is slightly on top of the previous form. The translation of the form downwards and to the right each time gives the figure the exact sense depicted by the painting’s title.

Eadweard Muybridge was a photographer who took many photographs of moving objects with a very fast shutter speed, and then placed each image succinctly in a row. His experimentation with photography was the first evidence that when horses ran, all four feet were in the air when they galloped, rather than the previous belief that one foot was always on the ground. Although each image separately shows a still of a horse and rider, when combined as a series, the photographs become movement oriented and show the progression of over time.

Harold “Doc” Edgerton pioneered a new form of photography where his camera was able to capture events occurring at such high speeds, it is invisible to the naked eye. Within this one frame, the cause and the effect is captured, and although the photograph is singular, the image still has a sense of movement due to the precise moment of the image within the overall process of the bullet being shot through the fruit.
To the left is the first draft of creating a notation system. Here, I was very focused on what went into the reaction at each step as well as what products came out at each step.

As seen in the drawn reaction on the previous page, there are changes to the molecule with each new enzyme, and a new transformation of the original glucose molecule is seen at the next stable state.

The shape as a whole represents one molecule of glucose; each square is an atom, red=hydrogen, blue=oxygen, and green=carbon. Yellow represents a catalyst which attaches to certain atoms in the reaction to perpetuate a change, then leaves the reaction.

This purple strand of atoms represents ATP which is a molecule of energy.

This version was my most detailed visualization showing the process the molecule went through during the reaction. I introduced transparency to show the separation between stable states and the brief intermediate states that the molecule formation was in, as well as different arrow types to show when the enzyme and energy enter and exit the reaction as opposed to the dotted arrows showing the transition of the glucose molecule between states.
At this point, I created my system of rules by which I finalized my square notation system. Bonding locations are represented by the connection of two white squares. Most often, four bonding locations is the most an atom can stably attach to at one time.

Each colored and black square represents an element in the periodic table, and the colors are based on the CPK color system developed by Corey, Pauling and Koltun in the 1950’s as a standard for molecule coloring.

If the two atoms share a double bond, they are connected by double the number of electrons and thus much stronger.

This version is more similar to the bond-line notation form seen in previous examples where the bonds are exterior to the element. My final method placed the bonds internally to the element. The bonds still visually separate the different elements, but the same amount of information is visualized in a smaller space.
The enzyme Helokinase enters the reaction and attaches to the hydrogen. Helokinase pulls the hydrogen off of the oxygen, leaving it unstable. Helokinase exits the reaction unchanged, and the hydrogen leaves the reaction.

ATP (adenine triphosphate) is attracted to the unstable connection end of the oxygen and attaches.

To the left is a detail of the final version of the reaction. The molecules are represented as square forms with points of attachment. The full opacity atoms show stable states, or areas of interest where as the transparent parts show intermediate states as well as parts of the molecule that are not changing. The curved lines were chosen as a response to the previous version where the lines were angular. These give a distinction away from the angular shapes. The unstable atoms are seen as molecules in motion where they have some overlay to imply vibration and movement.

ATP, however, is not stable when connected to the oxygen and the rest of the molecule. ATP breaks apart, leaving one phosphate molecule attached to the glucose, and ADP (adenine diphosphate) leaves the reaction. The molecule of glucose is now stable again and is called Glucose-6 Phosphate as it has the addition of the one phosphate molecule.
For the remainder of this project, Oxidation of a Primary Alcohol will be the reaction used as a basis for all visualization work.

Oxidation is the addition of an oxygen atom to a molecule. A primary alcohol is any molecule that has an oxygen atom and a hydrogen atom (-O-H) connected to one end of the molecule.

This oxidation reaction is very easy to identify, and I will be following it through a series of reactions until an aldehyde is created.

An aldehyde (in the red circle) is a molecule that has an oxygen connected by a double bond, and has two other connections where one connection is a hydrogen. Fulfilling these two requirements means that a molecule is an aldehyde.
To perform an oxidation reaction, an alcohol must be present. Here we see a molecule of a primary alcohol. Another oxygen enters into the reaction. The two hydrogen atoms have a greater attraction for the new oxygen than they do to their current bonds. The new oxygen pulls the hydrogens off the molecule. With the hydrogens gone, the atom of oxygen and hydrogen are both unstable. The two unstable atoms bond to each other and re-stabilize through a double bond. As an aldehyde. One molecule of water is formed between the oxygen and two hydrogen atoms.

using the square notation system

This visualization of the oxidation of the primary alcohol is seen using the square notation system developed in this chapter. One difference is that there are more steps seen here in the bond-line form than in the square notation. The available intermediate steps in the reaction as well as the stable and unsplit.

To perform an oxidation reaction, an alcohol must be present. Here we see a molecule of a primary alcohol. Another oxygen enters into the reaction. The two hydrogen atoms have a greater attraction for the new oxygen than they do to their current bonds. The new oxygen pulls the hydrogens off the molecule. With the hydrogens gone, the atom of oxygen and hydrogen are both unstable. The two unstable atoms bond to each other and re-stabilize through a double bond. As an aldehyde. One molecule of water is formed between the oxygen and two hydrogen atoms.
Chemistry is a body of concepts that is represented only through abstracted drawn notations or through 3D images that represent the atoms and molecules. But what is chemistry? Chemistry is composed of the interactions that occur between two or more molecules, and those interactions are either permanent or reversible. Chemistry is also extremely dynamic as it proceeds through a reaction as energy is lost or gained and the molecule either breaks apart or fuses together. Visualizing these interactions is very difficult though as we cannot actually see chemistry. The hand-drawn notation methods all have representations of the stable states, in between each state is an arrow, and the process is depicted as distinct systematic steps. I was inspired to think about methods that can bring the context of these reactions into a real representation that can be physically seen, and to translate the components of chemistry into real-world components that relate to our scale of representation.

I chose dance as my medium by which to "perform" the chemical reaction. Each body represents an atom, is colored coded to match the CPK system, and each body also has a place in the overall human-made molecule.

There have been other examples where artists and designers have used the ideas of atoms and molecules as inspiration of creating real world objects. Bringing chemistry into the macro-scale brings a sense of familiarity with the shapes regardless of the subject—matter.

Particle by Sara Ivanyi explains this project as “thirteen separate wooden parts that can be arranged like the atoms and bonds that make a citric acid molecule. Fruits become the atoms in their own molecular component in this design as citric acid connects all fruit.”

Brighter Minds by Felix Patone is a collection of lamps that are inspired by molecules where the “atoms” are the lit bulbs and the “bonds” are the metal connections.

Fondly t:Y) have been keenly portrayed the phrase as “human separate molecular parts that can be connected together and become the shape and translation. Fruits become atoms in this new molecular configuration in the design of a real-world component of light.”

Brighter Minds by Felix Patone is a collection of lamps that are inspired by molecules such that “the atoms” are lit bulbs and “bonds,” are the metal connections.
The Atomium is a building built for the 1958 Worlds Fair in Brussels. It was designed by engineer André Waterkeyn and architects André and Jean Polak.

Davide Tonizzo created the Molecule Seating System for the Canadian furniture company Arconas. It is composed of two heights of cylinder seating pieces that can be fit together into an infinite number of combinations and lengths.

The reaction performed by the dancers is the same as the reaction shown earlier. It is important to note that this reaction is part of a larger overall reaction. Certain facets of the chemistry have been simplified for proof of concept as well as because of the limitation of dancers. This project is concerned with oxidizing the alcohol one step to the aldehyde, but one could imagine this reaction proceeding completely until the aldehyde becomes carboxylic acid.
Atoms come together to form a molecule by creating bonds. Bonds are a pair of electrons that are shared between two atoms, thus because they are shared, they remain physically very close to one another. Each atom has electrons, but the number of shareable electrons vary by element. Looking at all the visual types thus far, these bonds are commonly visualized as a line showing the connection between two atoms.

Bringing this connection into a macro-scale representation, the dancer’s arms will serve as the bonds, and they can connect to other dancers through physical connections. Having a flexible connection also allows for bonds to easily be broken, and with broken bonds comes moments of extreme instability. Using a dancer as the medium, allows for these moments to be brought to life. Through a blend of techniques, the two dancers are left with an unbalanced feel that clearly is looking for a place of attachment. Bringing these moments into our scale of understanding can help us form a mental model of how the reaction actually proceeds.

Here is the first draft incorporating dancers as molecules into the reaction. Each dancer will have a way to connect and be part of the larger, overall molecule. These diagrams are references for the “states” that the molecule, but it is up to the dancers’ improvisation to see how they will embody their specific atom, how they will interact with other atoms, and how they will break old bonds and form new ones.

The hydrogens have switched, and have formed a water molecule with the new oxygen atom. this leaves Carbon #6 and Oxygen #7 unstable and without a connection.

Dancer #10, a oxygen, enters the reaction. The two hydrogens closest to her are now being drawn to her more powerful attraction and away from the alcohol molecule.

Each dancer is given a number which corresponds to a numbered atom in the reaction.

The unstable dancers realize they can form a double bond with their two unstable, unconnected arms.

The dancer molecule is now stable and a double bond is formed between dancer #6 and #7 creating the aldehyde.
An identical primary alcohol as the square notation is seen here.

Oxygen enters into the reaction on the right hand side.
The two hydrogen atoms are drawn to their strong attraction in this molecule. The oxygen's strength pulls the two hydrogens away from the original molecule. This leaves two bonds with no connections.
The oxygen double bonds both arms to the carbon as a way to re-stabilize. A molecule of water is formed with the oxygen and two hydrogens.
Looking at all three methods of representation simultaneously, comparisons and differences can be seen across the three. Different visual languages have different goals and thus the information seen changes between them. Chemistry is a challenging subject to visualize because we are incapable of rationalizing the sizes and shapes in our scale of life.

Using dancers as a medium for a chemical reaction not only creates a truly visual language we can see, but it also gives us a way to see the dynamics of the chemical reactions and then translate it back to a still two-dimensional image or representation. These dance images are part of a larger video where the dance was actually performed, and simultaneously seeing the performed dance reaction alongside the reaction performed with the notation gives rise to a new visualization type where each visual language works congruently with the other and creates a multi-layered way of understanding the reaction.

Viewing these steps at the same time works to showcase different visual representations as facets of the whole reaction. Next we will explore the depth of this multi-layered visualization, and how the parts can exist as complements to each other to assist understanding.
First: the model must enhance a feeling for—and not distort understanding of—the reality behind the communication by limiting its content ends to clearly apparent objectives.

Second: the design analysis of the model must be motivated by a devotion to clarity to assure that its three-dimensional form is the most economical, time-saving and meaningful way to convey the information.

Third: organization and translation of data into space, scale, material, form, color motion, sound or timed sequence must result in such a simple yet intense sensory and logically structured experience that the model is easy to remember.

Will Burtin, Thoughts on Three-Dimensional Science Communication
The ability to really see something is due, in part, to the ability to approach the object from different perspectives. To understand shape fully, one must have the sense of approaching it from all sides.

An example from the past that investigates this same idea of visualizing material from multiple views is seen in Rudolf Arnheim’s *Art and Visual Perception: a psychology of the creative eye*. Here Arnheim shows a chair, and then drawings a, b, c, and d show the same chair from different perspectives. The four sides do not look related unless the viewer understands that the subject matter is a chair.

This same principle applies to understanding chemical molecules and their reactions. It becomes easier to understand a certain perspective of a molecule when there are other visualizations that show the same molecular structure from a different perspective. Understanding chemical structures together as a cohesive set to give a better overall visualization of the single chair.

Multiple views of the same information have become common in many aspects of everyday life. The best capture is in our cars, as we see a map folding dozens of information on a single screen. The current step in the directions, but also an overall overview of our positions within the bigger map of the space. The car navigation directions have a split view of the next turn in a person’s route and the overall map of the city. The different perspectives give a different kind of information within one image.

There are many different types of learners. Some students learn best by linguistic means such as saying, hearing, and seeing words. Others are logical learners and learn best by working with categories and abstract patterns. Spatial learners work best with visual pictures and colors. Some students are kinesthetic learners and they learn through movement and interactions in their environment. Other students are interpersonal learners and they learn through group activities and the intra-personal learners are often most successful when working by themselves in their own space.

Although there are many different types, often students are a combination of a few. Throughout this process I was very focused on creating a system of representations that can assist a wide range of learning styles, and this unified system of chemical representations is my contribution to the broken visual circuit often seen in the subject.
Here are two pages from Oliver Byrne's *The First Six Books of the Elements of Euclid* written in 1847. Here he took the geometry ideas created by the mathematician Euclid in 300 BC and transformed them into visual and colorful components where the small pieces can be placed together to better understand the whole. This is one of the oldest examples of color and small visualizations used to try to better understand the subject. Byrne's investigation was a catalyst for this thesis project as geometry and chemistry share many similarities on paper: both are usually hand drawn, flat or simple perspective, and use only black line. Changing the standard, however, Bye is able to use color in order to simplify the complex, and use color as dividing the whole image into components.

Chemistry is a subject that is simultaneously visual and not visual at all: humans cannot see atoms and bonds in the real world, so the only way to understand the subject is through visual representations. This thesis project is a way to investigate the current systems in place for chemistry notations and representations. Although chemistry is a dynamic and multi-faceted subject, I felt strongly that the different types of representations all stemmed from the same core ideas and rules. The paradigm with chemistry was not a way to demystify chemical reactions but components that are not simple shapes, but rather forms that can embody the dynamic nature of the atoms.

This system of multiple representations is meant to be lead based however a student might feel. The goal is to present a group of different visual tools that all represent the same natural but otherwise different.

In summary, chemistry has always had many different types of representations. It is a visual challenge that has not gone unattempted. However, it has not been attempted this way. Combining different scales, flat, tangible, and dynamic forms, this thesis project is a new view on different visual notation representations of chemistry.

Throughout all these notation visualizations, the original form is also important to consider. The bond-line formation is most well known across all levels of chemistry, and its representation should not be discredited. This is a form that still lends itself to hand drawing, and is one of the most common forms used on chemistry tests as a way to test a student's understanding of the subject.

This thesis project, Thoughts on Visualizing Chemistry, is simply that; thoughts on visualizing this subject. Each visualization technique has benefits and disadvantages and so it is hard to make claims that one is superior to the other. It can be claimed, however, that multiple representations of the same material provide a better understanding of the subject than a single one.
Creating a new notation method was a way to look at the current ways of how chemistry is being notated and to propose a new system that visualizes it differently. One facet that I felt very strongly about is that color should play an important role. Color has the ability to categorize information easily, and using a colored notation system would help reinforce the material. As described before, squares seemed like a logical choice as the corners represented bonding locations and the shapes themselves fit together to form very geometric and patterned forms.

The square notation

One benefit of this notation is its ability to visually show instability and movement through transparency and overlay. As seen here, the two hydrogens disconnect. Considering the past examples of static depictions of movement, this representation gives those two atoms sense of jittery movement.

As a whole, this notation system can vary from a limited number of tiles to using all of the shapes themselves to form very geometric and patterned forms. Adding animation allows the squares to function in a new dimension where their dynamic movements can be seen within the new dimension of time.

The tiles

The tiles are ways of building molecular structures. Stemming from the square notation is a system of three-dimensional tiles that could be used to build molecules. The tiles are made of building CPK color system, and the corners have spots for Velcro-attachments. The set also has smaller white pieces that can Velcro on top and when two squares are lined up corner-to-corner, bonds form. Working with these geometric pieces helps the student understand how many bonding locations are available on each piece as well as how two atoms share and break bonds.

The dance

Although seen throughout this book as images, the choreographed chemical reaction also exists as a video set to instrumental music. The benefit of this form is that the reaction is not only in actual motion, but the entire process becomes more relatable as it is visualized with humans. Increasing from atomic scale to human beings representing atoms is a way to make the concept more understandable. The dance also becomes the most successful way of showing the dynamics of certain atoms when they have brief moments of instability. Depicting motion and dynamics is still a very challenging task, but coupling a dynamic video with static representations is a solution to better understand how atoms are actually interacting.
Looking to the future, I believe that the visual techniques used to explain chemical reactions will continuously improve. Using this method, I believe that there is room to improve and expand within the digital learning object field. Currently there are many different online and gaming-platform tools that are used to facilitate learning and the understanding of material for students. Taking the dancers out of the videos and into an educational gaming environment, this proposed way of understanding could be converted into an experience similar to the group sports games like Madden. Students could build reactions using the square or bond-line notation (plays) and then see the reaction in the box as they build the reactions, either in the captions (announcer) while watching how the reaction they built is danced with the virtual characters. Adding the level of the students participation in building the reactions could continue to evolve this system and provide another way by which students can study and understand the material.

Graphic designer and pioneer in scientific communication, Will Burtin once said, “To convey meaning, to facilitate understanding of reality and thereby help further progress, is a wonderful and challenging task for design. The writer, scientist, painter, philosopher and the designer of visual communication in commerce, are all partners in the task of inventing the dramatic and electrifying shortcut to a more comprehensive grasp of our time.” New perspectives of visualizations will be the way of forever evolving the way to understand these complex subjects. The key to successful designs is through collaboration of different disciplines and the combination of different perspectives.

Thoughts on Visualizing Chemistry is a way to showcase the wide range of visual possibilities in which information can be encoded, and that unlikely parallels in representation can work together to create meaningful visual information.