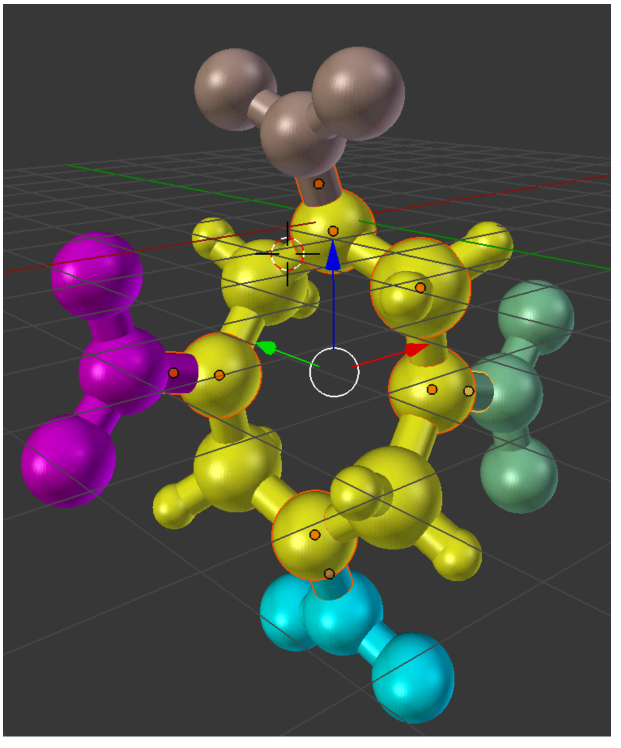

Printing 3D Models for Chemistry

A Step-by-Step Open-Source Guide for Hobbyists, Corporate Professionals, and Educators and Students in K-12 and Higher Education

Elisabeth Grace Billman-Benveniste
Jacob Franz
Loredana Valenzano-Slough

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Contents

I dedicate this book to the scientists, researchers, students, corporate professionals, and educators for whom these ideas are intended to benefit. I sincerely hope the methods we propose may aid in the development of chemical models capable of illustrating whatever science you are passionate about communicating.

-Grace

I dedicate this book to the open-source community; the hobbyists, engineers, programmers, scientists, and artists whose contributions made this work possible. Thank you for your time commitment, sharing your talents, and selflessly making your work freely available for the benefit of others in the community.

-Jacob

Dedicated to the dreamers who,
even when scared,
do not stop chasing their dreams.

-Loredana

About the Authors

Elisabeth Grace Billman-Benveniste

Grace is an alumna of Michigan Technological University where she studied chemistry, graduating with her B.S. degree in general chemistry in the spring of 2019.

After completing her undergraduate degree in chemistry, Grace has decided to continue her education in the accelerated Master of Business Administration program at Michigan Tech (graduating in the spring of 2020) with the goal of taking on leadership roles in industry.

Having been a student in several chemistry courses, a teaching assistant for university chemistry and quantum mechanics labs, and an undergraduate researcher in Dr. Valenzano's research group at Michigan Tech, Grace has a unique perspective in the application and efficacy of 3D-printed chemistry models in collegiate classroom and research environments.

After spending a summer working in a research-based metallurgical laboratory at a leading global gold mining corporation, Grace also has valuable insights into potential advantages of implementing chemistry models in industry.

Outside of academic work and involvement, Grace enjoys cooking, baking, painting, quilling, crocheting, and a variety of outdoor activities including hiking, camping, canoeing, gardening, and preserving a variety of foraged fruits.

Jacob Franz

Jacob is a mechanical engineering student at Michigan Technological University.

After completing his B.S. degree in mechanical engineering (graduating in spring 2020), Jacob is planning to continue his education in the accelerated Master of Business Administration program at Michigan Tech (graduating in fall 2020) in hopes of taking on leadership and upper management roles in industry.

Although Jacob enjoys many facets of mechanical engineering and manufacturing, he is most interested in additive manufacturing processes including 3D-printing. As a member of the open-source hardware enterprise at Michigan Tech, 3D-printing undergraduate researcher in Dr. Valenzano's research group, Co-Op student at a manufacturing company, and a digital fabrication hobbyist in his free time, Jacob has developed a strong knowledge base in 3D-printing technology.

Jacob also strives to always uphold the open-source philosophy which has allowed 3D-printing technology to grow very rapidly compared to other technological developments.

In addition to his interest in digital fabrication, Jacob enjoys woodworking, playing broomball and hockey, participating in Michigan Tech Pep Band events as a percussionist, and a wide range of outdoor activities including mountain biking, snowboarding, hiking, and canoeing.

Loredana Valenzano-Slough

Loredana is currently Associate Professor in the Department of Chemistry at Michigan Technological University.

In 1999, Loredana obtained her MS in Particle Physics from the University of Turin (Italy) in collaboration with the Stanford Linear Accelerator Center (SLAC, USA). She then moved to Southampton (UK) where in 2003 she obtained a Ph.D. in Theoretical Physical Chemistry. For the next two years she worked as a postdoc at the Leiden University (The Netherlands), and in 2005 she returned to the University of Turin as postdoc and instructor in the Department of Chemistry where she developed her passion for solid state physical chemistry and teaching.

In 2010 she joined the Physics Department at Michigan Tech as Assistant Research Scientist and Instructor. In August 2012 she was appointed Assistant Professor of Chemistry, and in Spring 2018 she was promoted to the rank of Associate Professor.

Loredana has published nearly 50 papers in peer review journals (h-factor=20), and she has presented her research all over Europe, the US, and most recently in India.

At Michigan Tech, in addition to regularly teach Physical Chemistry I, Physical Chemistry II, and Computational Chemistry, Loredana has developed three new courses: Math for Physical Chemistry I, Physical Chemistry III, and Quantum Chemistry.

When not busy at Michigan Tech, Loredana loves cooking, playing soprano, alto, tenor, and bass recorder, and training for her next ultra-marathon. Loredana leaves in the Upper Peninsula of Michigan with her husband William and their thirteen-year-old son Emanuele.

Acknowledgments

The authors would like to thank Michigan Technological University for generous support through the Research Excellence Fund initiative (REF-R01468). The Chemistry Department at Michigan Technological University is acknowledged for lab space.

Those who provided their honest feedback and testimonials are recognized for their contributions as well: Andrew Galerneau (Michigan Tech Senior Lecturer in Chemistry), Amanda Studinger (Former Northern Michigan University Chemistry Instructor and Current Chemistry PhD Student at Michigan Tech), Peyton Bainbridge (Michigan Tech Chemistry Undergraduate Student).

The authors would also like to thank members of the open-source 3D-printing community for dedicating their talents and enthusiasm toward designing, programming, and sharing their technical knowledge to the advancement of 3D-printing technology. This work would not have been possible if it was not for the supportive and collaborative environment embraced by the 3D-printing community.

Last but not least, one of the editors of the ACS Journal of Chemical Education is acknowledged for judging this work not suitable for publication in his journal; his decision initiated the editing of this book which the Authors are immensely proud to share with those passionate about teaching and learning.

"Every problem is an opportunity in disguise."

-John Adams

Founding Father and Second President of the United States of America

Testimonials

"In my previous years of teaching solid state and unit cells to my students, I had previously used a model that I had crafted from a Tupperware container and an old molecular modeling kit. The former model enabled me to communicate stacking patterns, but the combination of small spheres and the walls of the container made it very difficult to work with and project using a document camera to a room of 250+ students. The 3D printed model provided not only a larger scale (greatly enhancing visibility) for demonstrating stacking patterns, but the fused components also enabled me to pull out and remove a face-centered cubic (fcc) unit cell to demonstrate the three-dimensional origin from the a-b-c stacking pattern.

In previous years of teaching University Chemistry II, I also did not have access to an adequate model for the cut-away fcc unit cell and the rock salt unit cell. Previously, I had to rely on static images from the text book and cartoon drawings of the unit cells that I would produce in class. The two 3D printed models were essential for communicating and demonstrating the location of the two different types of interstitial spaces found within those crystal lattices, especially when used with i>clickers quiz questions. The models were also very helpful after class and during office hours by enabling students to physically hold a model and refer aspects of it directly.

In regard to direct student feedback on my use of the models last semester. I received the following excerpts of responses to the question, "As I, the instructor, prepare to teach this class again, what aspects of this course (teaching methods, assignments, areas of emphasis, etc.) should I preserve that effectively furthered your learning?":

- *"The 3D models helped a lot and this should be preserved.";*
- *"Those 3d printed models were helpful as well.";*
- *"The 3D printed models of lattice structures were very nice."; and*

- *"I would suggest having more physical/visual demonstrations such as the 3-D Models that were brought in towards the end of the semester"*

That final statement really struck home the value of physical 3D models for classroom demonstration. I believe digital models have their place in a classroom too, but for my part there is something important about the tactile interaction with a physical object that can really engage a learner. In particular, this is important for a discipline like chemistry where we deal so frequently in the abstract or material which is not immediately visible. I look forward to the increase use of physical models for select concepts in a general chemistry curriculum. Furthermore, I think there would be a lot of value to having a small collection of these models available for group work in either a recitation or Supplemental Instruction (SI) environment."

Andrew Galerneau
Senior Lecturer and Lab Supervisor
Department of Chemistry, Michigan Technological University

"*During my undergrad as a chemistry major, trying to wrap my head around the three-dimensional shapes of chemical molecules, their symmetry, and how they overlapped and stacked on top of each other was quite a daunting task and one that started in my first general chemistry course and continued to build in complexity all throughout my undergrad.*

It was not easy to try to visualize the difference between a face centered and body centered cubic unit cell when all we had at our disposal were dots and lines on a chalk board, let alone try to understand how the structure had an impact on the physical properties of the overall crystal. Many hours were spent watching my professors try to demonstrate

molecular packing with a piece of chalk in one hand and as many hand contortions they could muster with the other to try to demonstrate how molecules interacted with each other.

Later in life while teaching college chemistry, I understood the frustration and confusion my students were feeling as I was trying to describe crystal lattice structures. While ball and stick models help students build molecules, and beads and Styrofoam balls can be used to try to build a cubic unit cell, it is still a difficult concept to teach to students, especially when they are expected to not only understand the geometry but also how that geometry affects physical properties.

The first time I saw a 3D printed cubic unit cell, I couldn't believe how clear and easy it was to see molecular packing. I could hold the model from any angle, see how each molecule overlapped, and see and feel the voids that were created from the specific packing of the cube. It was easy to see how a tightly packed cubic unit cell would have stronger intermolecular forces in the crystal lattice structure and how other atoms and molecules could nestle in the voids and have an impact on the overall stability of the structure. I wished I had a model like that for my class! Having 3D models of complex structures where students can touch and rotate, pull apart and put back together is an amazing asset to have in the classroom.

I know that from my own experience as a student and later as a teacher, having the opportunity to work hands on with a theoretical concept would make 3D printing a priceless teaching and learning tool!"

Amanda Studinger
Former Northern Michigan University Chemistry Instructor
PhD Student
Department of Chemistry, Michigan Technological University

"Even in the first couple classes of any general chemistry courses, the phrase, "Chemistry is the building blocks of life" gets thrown around. Electrons, protons, and neutrons are thrown around as givens in any early class, but a true understanding of these particles does happen further on. Quantum chemistry does give that in-depth look on something ironically, we cannot see.

My experience in a quantum chemistry class was very interesting. As one cannot see the nanoscopic systems, visualization was not my strong suit. This was a very big challenge in understanding the motion of electrons. With the help of a physical element, like the angular momentum 3D model, the understanding of these abstract ideas was much easier to achieve. I feel that without the 3D models more studying time would have been necessary to first internally understand the system and furthermore connect the theory behind it. I also do believe that these techniques of modeling can help in primary and secondary school. Overall, 3D modeling can be a connection for students into a world that we cannot see."

Peyton Bainbridge
Undergraduate Student
Department of Chemistry, Michigan Technological University

"*Thoughts on the 3D-printed vector model of the atom:*

- *I personally felt the use of the 3D-printed vector model of the atom was very beneficial in my physical chemistry (quantum mechanics) course. The vector model of the atom is very useful when learning about angular momentum, however I found it was very difficult to interpret and understand the model when provided as a two-dimensional figure in textbooks. I thought the 3D-printed model was far easier to interpret.*

Thoughts on a 3D-printed molecular model:

- *Using a 3D-printed polycarbonate fragment molecular model made all the difference during my research poster presentations. Several audience members made comments about how much they appreciated how they could easily visualize the molecule I was referencing and its various interactions through my use of the 3D-printed molecular model. Many of the judges also made comments about the model, unanimously agreeing it was a great addition to my presentation. During the second of two poster presentations I attended, I was awarded first place in the undergraduate poster presentation division, an achievement I attribute greatly to my use of the 3D-printed molecular model I used during my presentation."*

Elisabeth Grace Billman-Benveniste
Chemistry Graduate (BSc 2019), Michigan Technological University
MBA Graduate Student, Michigan Technological University

On the Several Motivations Behind the Book You are Holding in Your Hands

My primary research interest involves the quantum chemical computational characterization of physical-chemical properties of a broad range of materials. In my research group, scientific experimentation is conducted in silico through the use of state-of-the-art theoretical methods able to describe the electronic structure underlying the microscopic behavior of molecules, polymers, behavior at the interface, and crystalline systems. Various aspects contribute to the making of a successful and truthful theoretical/computational research project. Students in my research lab need to develop several skills; among others, they need to apply their chemical intuition to the understanding of the abstract mathematical nature of the underlying theories and approximations they are applying to obtain meaningful and original scientific results.

Among one of the most difficult skills I ask my student researchers to develop is the ability to visualize the three-dimensional nature of mathematical functions such as electron density and charge distributions, and how the molecules and materials they are investigating arrange in the 3D space. While software programs adopted include powerful graphical interfaces capable of showing three-dimensional physical-chemical properties and structures, when they are not accessible, as during poster presentations, conferences, and lectures, explaining abstract concepts and structural geometrical arrangements that develop with respect to a three-dimensional orientation using two-dimensional images can be very cumbersome and ineffective, especially to an audience not used to such topics. In these regards, the non-customizable nature of conventional 3D-modeling kits and high cost of custom ordered molecular models led to the idea for a new method of acquiring the visual representations my group needed: manufacturing our own models.

To begin our journey in the creation of custom atomic models, we enlisted the help of Jacob Franz, an undergraduate Mechanical Engineering student incredibly knowledgeable in the operation of 3D-printers and

capable of using all the necessary complementary software packages. Through many hours of research and tinkering, Jacob was able to create a full step-by-step procedure for the creation of custom molecular models. The first molecular model we successfully printed for further use in the research group was a molecular fragment of polycarbonate. Elisabeth Grace Billman-Benveniste successfully used the polycarbonate 3D model as an aid to visually describe the effect of water on a polycarbonate interface for her quantum chemical study; for her work, she delivered a first-prize winning presentation at the 2018 ACS Upper Peninsula Local Section (UPLS) Student Research Symposium at Northern Michigan University (NMU, Marquette, MI). Since then, we expanded the original idea to create other chemical models used in lower and upper-division undergraduate chemistry classes as educational aids.

Through the development and publication of this book, we hope to share our methods so others may also benefit from creating their own molecular models. Utilizing several open-source software packages, design engineering concepts, and 3D-printing technology, several straightforward methods were created, allowing individuals without any formal manufacturing or engineering training to produce fully functional 3D-printed chemical models.

This work is intended above all else to provide K-12 educators, academic and corporate professionals, researchers, and hobbyists alike with a handbook of procedures and ideas allowing for complete freedom and customizability of chemical models. Our methods and procedures were written with the goal of inspiring creativity and giving others all of the necessary tools to tailor chemical model designs, making them more functional, effective, and suitable for their desired use. We sincerely hope the examples we provide in this book will inspire others to explore the limitless number of possibilities for 3D-printing in chemical model creation.

In these regards, an additional important aspect characterizing our work is its complete adherence to open-source philosophy. This work was made

possible by the community of hobbyists, programmers, and tech-savvy tinkerers who worked tirelessly to create software programs, hardware, and firmware for which they expected no monetary compensation. The wealth of knowledge generated by the free sharing of ideas throughout the open-source community has led to an unprecedented acceleration of 3D-printing technological development. Through the publication of this book on an open-source platform, we intend to contribute to this wide breadth of knowledge.

We also hope our contribution may give back to the open-source community who paved the way and provided many of the tools my research group needed to create a better way of illustrating the scientific findings we are so passionate about sharing with others.

Last but not least, I personally want to publicly thank Grace and Jacob for their unlimited enthusiasm and passion in making all of this happening. Nothing of what you are going to read and learn about 3D printing would have been possible without them because, in all honesty, I didn't know anything about 3D printing until I started to work with them! I had some visions and ideas that I wanted to realize but I had no clue on how to make all of those becoming a reality. Well, Grace and Jacob made them into reality to the point that now I can touch those visions as 3D printed models.

-Loredana Valenzano-Slough

(September 2019)

Preface

In the past several years, hundreds of technological advancements have transformed 3D-printing from cumbersome and costly to efficient and highly profitable. Among other uses, industrial and academic organizations have implemented 3D-printing methods to manufacture valuable models. For example, 3D-printing may be used to produce prototypes or scaled models in industry and as visual aids for educational purposes in academia. In this work, we present a complete open-source step-by-step procedure for the conversion of virtual molecular structures to 3D-printable pin-and-hole style physical molecular models, a simple guide for model improvement, and unique insights into the limitless number of possibilities for 3D-printing in educational models creation. The models produced through the described methods and procedures can readily be used in both research and classroom environments and the proposed technology can offer an accessible and low-cost tool for schools, educators, and students at all education levels. Costs are further cut through the use of software packages, firmware, and hardware that strictly adhere to the open-source philosophy. Similarly, the software programs used are freely available to hobbyists, students, and educators and all designs for created models are made publicly available. The open-source aspect of the methods proposed herein allows for full customizability at every step of the model manufacturing process, not only in the use of the software programs utilized but even the 3D-printer itself. In addition, this work explains common practices for resolving technical issues generating failed prints; this aspect is stressed in an effort to curtail the fears of those who may doubt their ability to correctly diagnose and resolve 3D-printing issues and are thereby dissuaded from adopting 3D-printing technology.

Introduction

3D-printing is a relatively inexpensive additive manufacturing method used to create tangible objects. As a relatively new technology, the true capability of 3D-printing has not yet been fully exploited, especially in academic and research/teaching settings. Through this work, 3D-printing in a classroom and research environment is employed as a tool for creation of fully customizable, three-dimensional molecular models and for the visualization of theoretical abstract concepts.

While the idea of using 3D-printing as a method of producing highly customizable molecular models has been discussed for several years, to the authors' knowledge no other stepwise procedure adaptable to virtually all fused deposition modeling (FDM)-style 3D-printers has yet been proposed. While one 3D-printer manufacturer, Ultimaker, has developed a method for 3D-printing molecular models specifically using their company's 3D-printers and affiliated g-code preparation software packages, the described method may not be used on a 3D-printer manufactured by other companies and lacks some of the customizability incorporated in the procedures described in this work.[1] For example, Ultimaker's suggested method for 3D-printing simple molecular models in 2016 lacks the pin-and-hole feature, limiting the potential complexity of molecular models with no ability to take the model apart if so desired.[1] In fact, the pin-and-hole feature may be very valuable for a classroom or research environment to aid in understanding and stressing geometric features, steric arrangements, symmetry, and chirality of molecules among other logistical benefits.

Originally studied and documented prior to 1981, the mechanisms by which people absorb and remember information is very well understood.[2] As cited in countless educational literature studies, people learn through the use of their sensory organs according to the mechanisms described in Figure 1.[2]

Because an average of 94.0% of information is absorbed through the senses of sight and hearing, for most non-visual or hearing-impaired persons, the

use of models and visual representations when teaching, is expected to significantly improve learning capabilities. Furthermore, many studies suggest that the use of visual representations greatly increases the average information retention rate in adults without any sensory-affecting disabilities by an estimated 55% compared to verbal lecture alone when exposed to a new topic (Figure 2).[3]

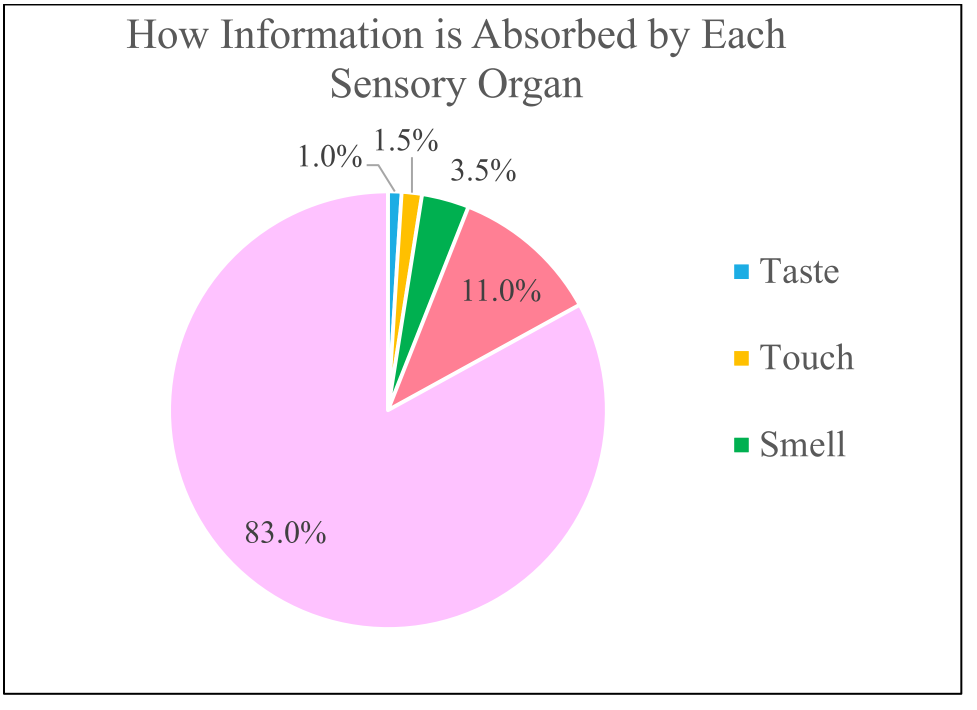


Figure 1: How information is absorbed by each sensory organ during active learning. This data is representative only of individuals who do not have any disabilities impeding one or more of their senses.[2]

Because an average of 94.0% of information is absorbed through the senses of sight and hearing, for most non-visual or hearing-impaired persons, the use of models and visual representations when teaching, is expected to significantly improve learning capabilities. Furthermore, many studies suggest that the use of visual representations greatly increases the average information retention rate in adults without any sensory-affecting disabilities

by an estimated 55% compared to verbal lecture alone when exposed to a new topic (Figure 2).[3]

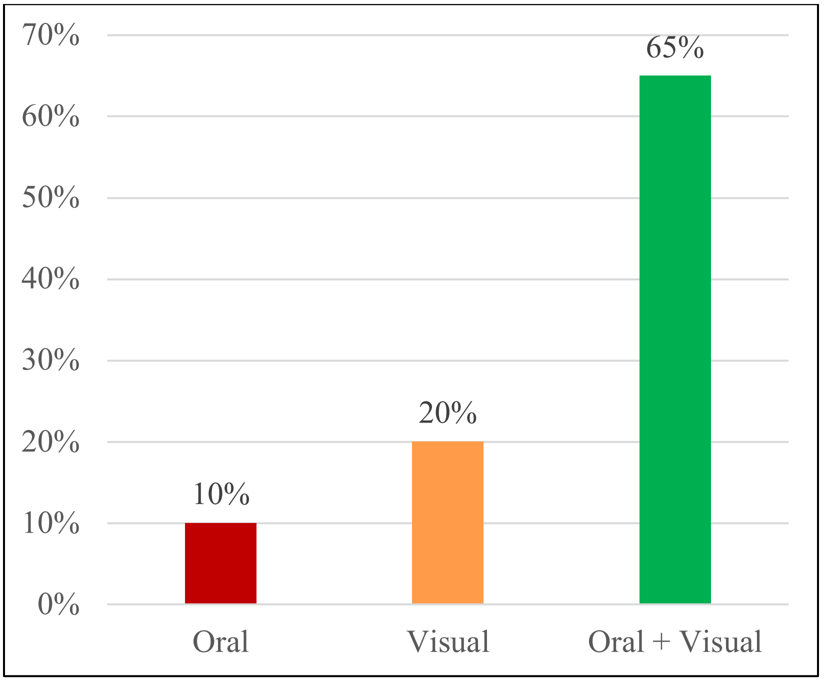


Figure 2: Retention of learned information 72 hours after oral, visual, or oral and visual presentation for non-visual or hearing-impaired individuals.

The benefits of using visual aids in education may become even more evident if the topic is inherently difficult to visualize; this is the case for scientific-related topics such as molecular and crystalline structures and symmetry, which of course cannot be appreciated with the naked eye and are not necessarily related to any daily experience that subjects develop in their formative years.[4-6]

While it has become clearly evident that visual representations can be quite valuable in education, educators are often reluctant to use them due to issues of cost and inaccessibility. It is easy to understand why, for example, a chemistry instructor may wish to explain the geometry of a non-planar molecule using a three-dimensional model as opposed to the

canonical approach of a two-dimensional picture or drawing on the board. To do so, the instructor would either need to purchase a potentially expensive molecular model set including all of the atoms needed or pay a substantial fee for an outside company to design and produce an injection-molded model. In many cases, costs would be too high and/or the needed model too obscure for the production of educational models to be feasible. As a low-cost, customizable manufacturing tool, the technology and procedures proposed in this work for creation of visual representations is expected to have a greatly positive effect on awareness and accessibility for educators.

In this work, in addition to developing a full procedure for building 3D-printed molecular models, several specific design-enhancing techniques are discussed in detail as well as suggestions and ideas used for model improvement during the designing phase. One of the objectives of this work is to make the interested community aware of the customizability of 3D-printed molecular models and how using the proposed method is as limitless as the designer's creativity and imagination.

Hardware/Software Equipment and Operational Methods

The procedure outlined in this work requires access to both a 3D-printer and a computer capable of running all the required software. The minimum requirements of the computer (in order to run the necessary software efficiently) are a 32-bit dual core 2Ghz CPU, 2 GB RAM, OpenGL compatible graphics with 512 MB of RAM. Software packages used (described in detail later on) include Chimera[7], Blender[8], MolPrint3D[9], Slic3r Prusa Edition[10], and Cura Lulzbot Edition[11]. In the interest of the most flexibility, all of the software used are available for PC, Mac iOS, and Linux operating systems. For implementation of design-enhancing techniques, Fusion 360 (manufactured by Autodesk) was used.[12] While not technically open-source, Fusion 360 design software is freely available to student, educators, and hobbyists and has significantly greater capabilities than FreeCAD, an open-source design software option.[13]

The 3D-printer used for this project was an FDM-style 3D printer, the Lulzbot Taz 5 (Figure 3), manufactured by Aleph Objects.[14] The Taz 5 is an open-source machine; all of its design files are available for free on the Lulzbot website. The print area of the Taz 5 is 298 mm x 275 mm x 250 mm equipped with a heated borosilicate glass bed and a stock Polyetherimide (PEI) surface. The PEI surface is excellent for printing relatively large molecules in one print as it provides for an adequately strong adhesion to the print bed. It is capable of printing layer heights from 0.050 mm to 0.500 mm; this feature is particularly important when printing spheres, as the smaller the layer height, the more rounded the final object will feel and look.

FDM-style machines are the most common desktop 3D-printer currently available. Other styles of 3D-printers such as stereolithography (SLA) or selective laser sintering (SLS) machines are capable of achieving higher detail and printing in different materials. However, at the time of writing, both SLA- and SLS-style machines were considerably more expensive in comparison to the Taz 5 and other FDM-style machines. In addition to cost, there are several other significant disadvantages to the use of SLA or SLS-style machines. SLA-style machines rely on a type of resin that is unsafe to touch when uncured[15,16] and SLS-style machines use highly flammable and reactive fine metal powders.[16] Primarily for safety concerns, SLA and SLS-style machines should only be operated in dedicated rooms. Conversely, FDM-style machines such as the Taz 5 use relatively non-hazardous materials and generally do not require a dedicated space. FDM-style machines could easily be placed in a classroom, computer lab, or well-ventilated office and may be placed in an enclosure with air scrubbers if the desired material emits any unwanted fumes and odors while printing. While FDM-style machines are clearly the most appropriate for use in a classroom or lab setting for both affordability and safety, the Taz 5 was chosen in particular for its ease of use and balance between cost and quality of prints produced.

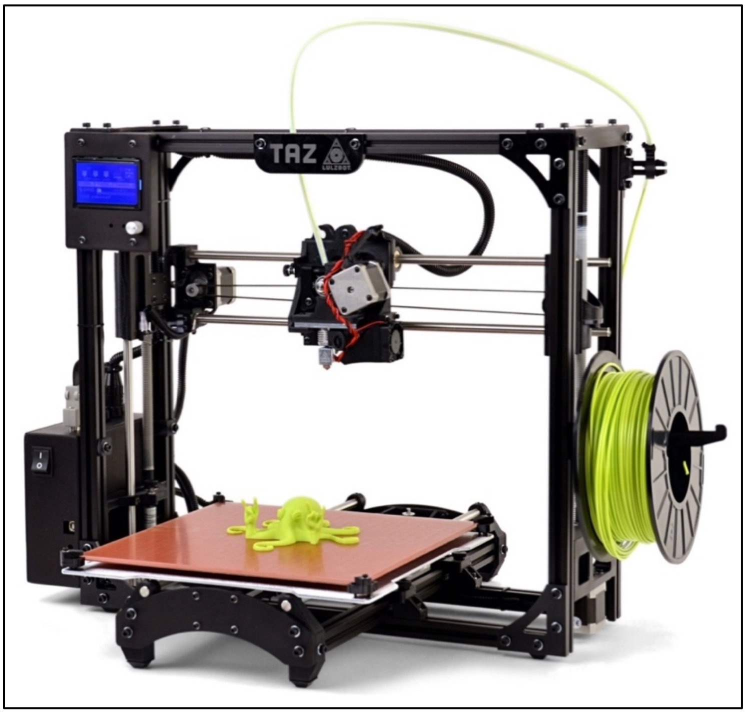


Figure 3: The Lulzbot Taz 5 3D-printer is shown above (image sourced from Lulzbot's official website).[14]

In Figure 4, a brief procedure for the customized set-up and calibration of the Lulzbot Taz 5 is outlined; nevertheless, the authors strongly suggest to follow the start-up instructions provided in the owner's manual when first calibrating a 3D-printer.[17] It is important to note that there may be slight variations in start-up procedure and calibration depending on the manufacturer and model of the 3D-printer used, however individualized calibration procedures are usually explained in details in the documentation provided by the 3D-printer manufacturer.

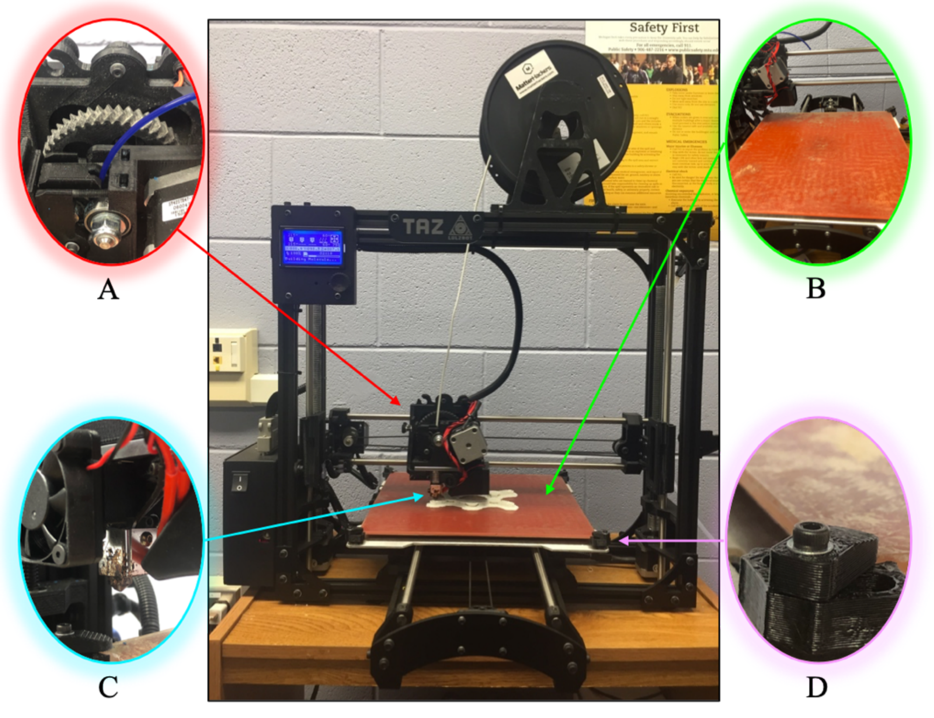


Figure 4: Several key features for set-up and calibration of the Lulzbot Taz 5 3D-printer are highlighted:

A) *The extruder assembly*
- *Make sure to inspect the extruder assembly before printing, as this is one of the most fragile components of the machine.*

B) *The heated borosilicate glass bed with a stock PEI surface*
- *Make sure to clean the surface with isopropyl alcohol before printing.*

C) *The extruder*
- *The extrusion rate should be adjusted until the proper amount of material flows through the nozzle.*

D) *One of four corner screws used for manual bed-leveling*
- *Use these screws to adjust the bed until it is not angled in any direction.*

After set-up and calibration, the printing material choice becomes a top priority. Many different types of thermoplastic filament are available for purchase, each with their own benefits and limitations. Overall, five different filament choices were considered: polylactic acid (PLA), acrylonitrile butadiene styrene (ABS), polyethylene terephthalate with glycol modification (PETG), thermoplastic elastomer (TPE), and polycarbonate (PC). PLA was chosen for building the models described in this work. The major reasons for this choice are the following: PLA tends to be the most reliable, easiest to print, safest (in terms of particle and fume emission) and the most cost-effective option among the materials listed above. Nevertheless, it is fair to stress that PLA does not possess the heat resistance and strength of ABS, PETG, and PC; in addition, it cannot be acetone smoothed (a convenient feature of ABS) and does not have the flexibility of TPE. Regardless, given the scope of this project, it was decided that the reliability and cost efficiency of PLA far outweighed the benefits of using other materials.

Common tools available at most hardware stores can be used to remove the printed object from the bed and to trim off any excess material (see Post-Processing Methods in SI). Typically, these tools are: (i) clam knife or paint scraper with rounded corners to remove the finished object from the print bed; (ii) sharp hobby knife such as an X-Acto knife for cleaning brim material around the base of the print and to remove excess pin material, improving the fit of joints when printing complex molecular structures; and (iii) flush cutters and pliers for removing support material and for preparing the filament for insertion into the extruder assembly. All of these tools are quite affordable and fairly self-explanatory for use in accomplishing their various tasks. The appearance and function of each tool listed above is provided in Table 1.

Table 1: A summary of each tool used for prying printed parts from the print bed, removing unwanted material from the printed object, trimming filament, and removing support material is pictured and described below. While the displayed tools were chosen for the purposes of this work, others may find a different tool more useful for their specific applications.

Tool Name	Tool Appearance	Tool Function
Clam Knife		Used to pry printed objects off of the print bed.
Paint Scraper		Used to pry printed objects off of the print bed.
Hobby Knife		May be helpful in removing unwanted or excess material from 3D printed objects.
Flush Cutters		Often used to remove stubborn or high-infill support material from 3D printed objects. May also be used to trim filament prior to insertion into the hot end assembly. Helpful for removing plastic after manual filament extrusion.

Pliers		*Used to remove support material from 3D printed objects.* *Cutting edge may be used to trim filament prior to insertion into the hot end assembly.*

Safety Procedures

Several safety precautions should be considered when 3D-printing and post-processing 3D-printed parts. 3D-printers should only be operated in well-ventilated areas such that any chemical fumes produced as the thermoplastic filament is melted are not inhaled, especially in the case of ABS.[18-21] The potential for thermal burns must also be considered when operating a 3D-printer. According to the manufacturer's website, the hot end of a TAZ 5 3D-printer can reach up to 305°C, most definitely hot enough to inflict painful burns. The hot end of any 3D-printer should never be touched directly before, during, or shortly after printing and care should be taken to only handle printed objects once they have cooled completely. In addition, it is critical to avoid moving parts while the printer is operating. Exposed moving parts create pinch points which may cause mechanical injuries. Mechanical injuries could also be sustained during removal of the 3D-printed object. When removing printed objects from the bed, it is quite often necessary to place a significant amount of force on the paint scraper. Once the object is freed, the paint scraper may rapidly continue down its intended trajectory, catching any ill-placed fingers in its path. For this reason, it is highly recommended to wear cut resistant gloves while removing objects from the bed. Cut resistant gloves as well as safety glasses should also be worn when removing excess material with any sharp tool. Children under the age of 13 should never operate a 3D-printer

unsupervised unless well-educated in the hazards associated with 3D-printing, how to avoid such hazards, and what to do in the case an accident does occur. Likewise, young children should never use sharp tools without adult supervision.

Proposed Method for 3D-Printing Pin-and-Hole Style Molecular Models

Figure 5 reports the flowchart containing all the steps necessary to build the final file (g-code format) used for printing the desired model. Using the proposed method, a molecular model of a polycarbonate fragment was created.

Molecular models were first created using the Gaussview 16 interface, the virtual molecular structure building tool the authors were most familiar with.[22] Although the Gaussview 16 software package is not free or open source, there are several other free molecular graphical interfaces available online including: Moldraw,[23] Avogadro,[24] Vesta,[25] Molekel,[26] Gabedit,[27] Jmol,[28] and Molden[29]. Virtually any molecular graphical interface may be used as long as the created molecule can be saved as a Protein Data Bank (PDB) file. In addition, molecular models may be sourced from online databases (including the CCDC) and saved as a PDB file format.[30, 31] In most cases UCSF Chimera[7] was used in order to convert the PDB file into either a stereolithography (STL) or virtual reality modeling language (WRL or VRML) file format.

After converting the files to the correct file format, Blender[8] was used to split the models and set up pins and holes. Blender is a very versatile opensource 3D modeling software that easily accepts numerous add-ons including MolPrint3D,[9] specifically designed for use in creating 3D printable molecular structures. Using the VRML file, the radius of each of the atoms and bonds within the molecular structure can easily be scaled up or down. The pin-and-hole feature may be used to break the molecule down into components at selected atoms and bonds which can be interlocked once the model is printed.

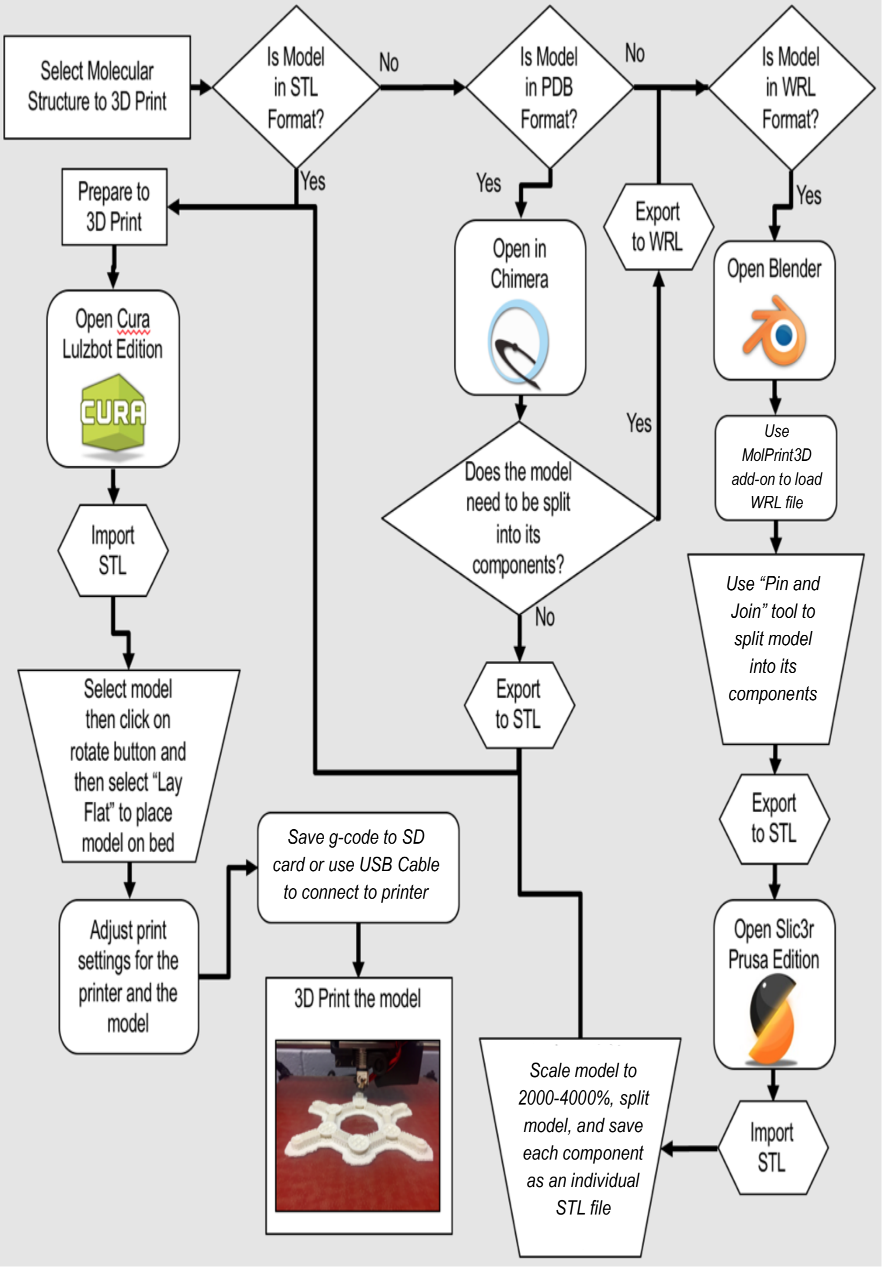
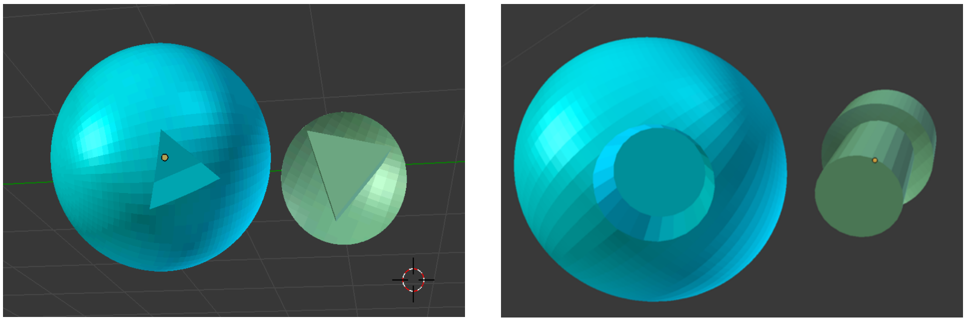


Figure 5: The flowchart above can be used to determine what software package should be used at each step of the g-code file preparation process.

The pins-and-holes have a scaling ratio to allow for manufacturing tolerance. If the tolerance is very tight, it is possible for the final model to sufficiently hold together by the force of friction alone. Strategically shaped

pins-and-holes may also aid in achieving desired inter-atomic angles within the molecular structure. For example, if a 60° angle is needed, a three-sided pin (i.e., an equilateral triangle pin geometry) would allow for a 60° rotation between the two components (Figure 6). Increasing the number of sides increases the roundness of the pin and if set to a high enough value may create a round pin with 360° rotation capabilities (Figure 6). At this point, it is necessary to use slicer software for separation of the various components and exportation as 3D printable STL files.



A **B**

Figure 6: A) A 3-sided pin-and-hole mechanism. B) A 25-sided pin-and-hole mechanism

Slicers are software packages that recognize the geometry of the object, split it into components, and output the model as a g-code file which the 3D-printer is able to interpret to print the model. Slicer settings also determine the temperature and speed settings of the machine and generate the support material (rafts) necessary for printing the molecular model. Appropriate temperature settings are vital, as different materials require different temperature settings for both the hot end and the heated bed and the speed may be adjusted as well to better accommodate complex models and materials which require slower printing speeds. Slicer programs are optimized for use with their respective printers and thus it is recommended that individuals new to 3D-printing use the printer

manufacturer's specific slicer package; however, it is possible to use virtually any slicer package the individual user is most comfortable with.

Two different slicers, Slic3r Prusa Edition[10] and Cura Lulzbot Edition[11] were implemented in this procedure. It is important to keep in mind that certain slicer packages offer useful features which may not be available in others. For example, although a Lulzbot machine was used in this work, Slic3r Prusa Edition was used extensively to scale and save each component of a complex polycarbonate molecule as an individual STL file. As individual files, the components could then be manipulated independently of one another, helping to avoid the addition of unnecessary support material by allowing for better orientation on the print bed or to print each component separately. Cura Lulzbot Edition does not have the capability of saving components of a single file as multiple STL files.

Slic3r Prusa Edition was also used to scale up the size of the model and to split the complex polycarbonate fragment model into components prior to saving each one as a separate STL file. Models were scaled up from a range of 2000% to 4000% depending on the purpose of the model to compensate for the conversion factor from inches (Blender) to millimeters (Slic3r Prusa Edition). When choosing the size of the model, the user needs to keep in mind that spheres tend to print more successfully as the model size is increased due to the greater surface area for print bed and layer adhesion. Finally, Cura Lulzbot Edition was used to prepare the model for printing via the Taz 5 3D-printer. Regardless of the slicer package used, the most important parameter to set (through much trial and error) is the inclusion of rafts for printing the molecular structures (Figure 7).

If rafts are not implemented, it is very unlikely the spheres of the molecule will adequately adhere to the bed, resulting in a failed print. If adhesion does occur, the bottom of the spheres may become greatly deformed when rafts are not implemented.

A summary of each software package used, its classification, and purpose is concisely summarized in Table 2. A more detailed tutorial-type description

for the use of each software program has been provided in the Tutorial (page 53 onward).

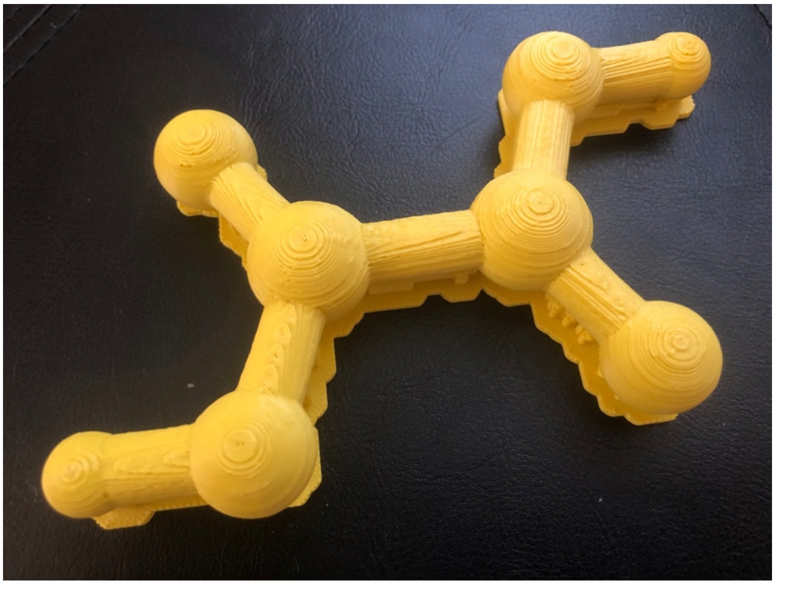


Figure 7: Support material (rafts) can be seen on the underside of the 3D-printed molecular model.

Table 2: A concise summary of each software package used, its classification, and purpose.

	Classification	***Purpose***
Chimera[7]	*File conversion software*	*Converts file format from PDB to STL, WRL, or VRML file formats.*
MolPrint3D[8]	*Add-on*	*Specially designed software for creating 3D-printable molecular models. Offers a pin-and-hole option.*
Open Blender[9]	*3D modeling software*	*Accepts MolPrint3D add-on. Also used to split the molecular model into its desirable components.*
Slic3r Prusa Edition[10]	*Slicer*	*Scales model and saves components as individual STL files.*
Cura Lulzbot Edition[11]	*Slicer*	*Arrange individual components on print bed and prepare the final 3D-printable g-code file.*

Using the proposed procedure, a fully functional 3D-printed molecular model of a polycarbonate fragment was produced. Snapshots of the polycarbonate model as it appeared in Blender, Cura Lulzbot, in components after printing, fully assembled, and fully assembled after painting are shown in Figure 8. Information regarding the painting process is outlined in the Tutorial (see page 53 onward).

This model in particular was used during poster presentations at scientific conferences to visually explain interactions between the double-bonded oxygen atom and several water molecules. The water molecules were also printed using this method.

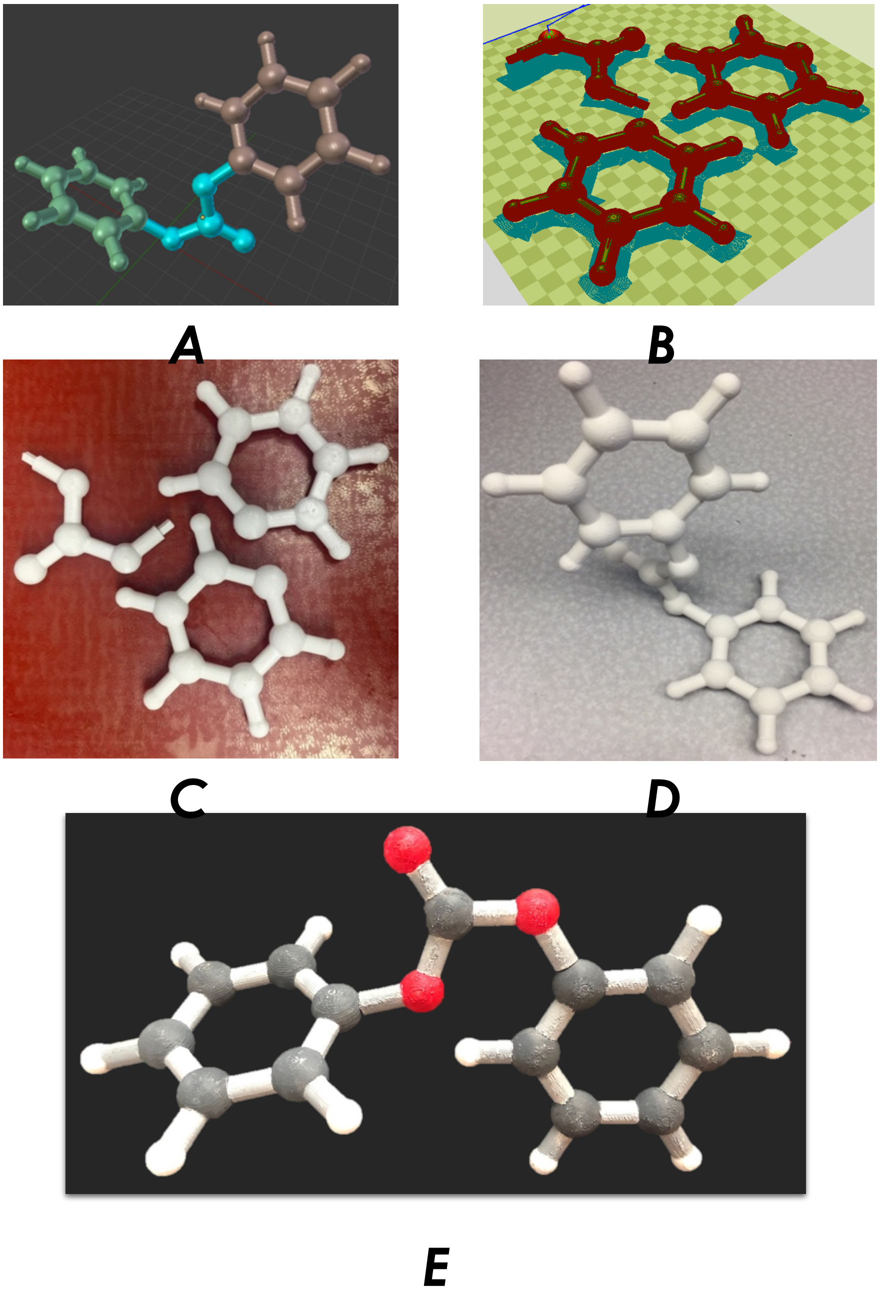


Figure 8: A) The molecular model viewed in Blender complete with pins and holes and ready to prepare for printing. B) The molecular model as visualized in Cura Lulzbot Edition in "Layer Preview" mode to view the model with support material. C) The molecular model as three separate components after support material was removed. D) The fully assembled model. E) The finished, painted and fully assembled 3D-printed pin-and-hole polycarbonate model.

3D-Printing Models for Advanced Topics (Quantum Mechanics)

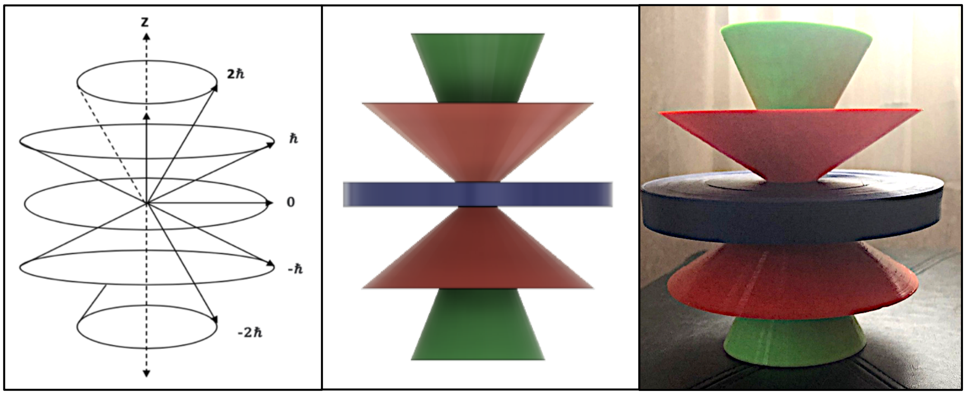
In most STEM-related higher education fields, students are expected to gain knowledge in various abstract mathematical and physical concepts. True understanding of such topics often requires spatial visualization skills in three dimensions which may be extremely difficult to conceptualize when taught using standard two-dimensional visual representations. Modeling of advanced curriculum using 3D-printing technology has the potential to drastically increase student comprehension of abstract mathematical and physical concepts by allowing students to visualize three-dimensional concepts in three-dimensional space.

In this work, the capabilities of 3D-printing to produce useful models in advanced topics was explored through creation of a 3D-printed vector model for the atomic angular momentum, a quantum mechanical concept typically covered in Physics and Chemistry undergraduate curricula. The vector model provides a convenient and practical representation of the complex mathematical relationships used to describe the angular momenta of electrons in atoms.[32] With respect to a 3D geometrical fashion, the angular momentum vectors for an electron located in a given atomic shell span the 3D space to form cone shapes of different radius and height. While the shape of the cone generated by the angular momentum vectors is unique for each quantum number, the apexes of all cones originates from the same points, as shown in Figure 9. The 3D-printed vector model of the atom (shown in its virtual and physical forms in Figure 9) has been used several times in quantum chemistry classes to highlight the resulting geometric nature of the complex mathematical concepts from which it originated. This valuable model gave students the opportunity to visualize the connection between related complex mathematical concepts and more easily conceptualized geometric outcomes of such mathematical principles.

In the first production of the 3D-printed vector model of the atom, a 3D-printed screw mechanism was used to adjoin all cones in the model,

however the screw mechanism unfortunately broke on several occasions when subjected to unacceptably low levels of force (Figure 10).

Moving forward, the 3D-printed screw will be replaced with a stronger metal mechanism, as used in the FCC unit cell model (see later). Note that before implementing 3D-printed hardware components comprised of metal, it is wise to perform preliminary tests to predict how easily the 3D printed component will fail when used for its intended purpose. In fact, for some applications, the force applied to the screw mechanism may prove too great for a plastic object to withstand.



A B C

Figure 9: A) The standard 2-dimensional angular momentum atomic vector model. B) The vector model of the atom as displayed in Fusion 360. C) The 3D printed vector model of the atom.

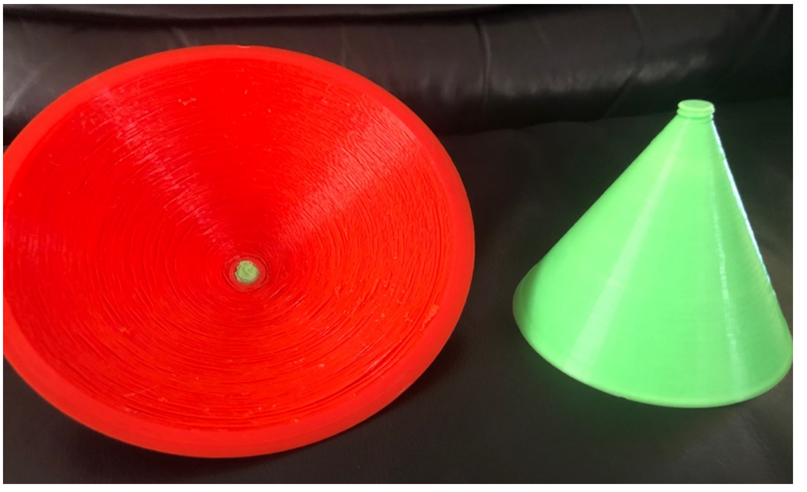


Figure 10: Excess material stuck in one of the cones as a result of the broken screw mechanism

Design-Enhancing Techniques

When creating 3D printable molecular models, it is vital to consider the overall functionality of the desired product prior to printing by answering the following questions during the design/engineering process:

- *Question 1: Are there weak points present in the current design? Could a portion of the model break off if not reinforced?*
- *Question 2: Can the model be broken down in a way that enhances its capabilities as an educational tool? What method would be optimal for putting the model back together?*
- *Question 3: Is there anything that could make this model better-suited for its intended purposes? What design elements could yield such improvements?*

Discussed below are several design methods employed to address each of these key questions for a specific project; building a series of unit cell models to use as educational aids in first year collegiate-level chemistry courses. This analysis should serve not only as examples of specific design-enhancing elements, but also to demonstrate how to use the three questions outlined above to design more useful 3D-printed models.

Teaching topics related to unit cells and crystal lattices pose several major challenges for both educators and students. The arrangement of atoms in a 3D unit cell structure requires an aptitude for spatial visualization and is quite difficult to express in two-dimensional space (such as an image in a textbook). In addition, the stacking patterns present in face-centered-cubic (FCC) and hexagonal-closest-packed (HCP) unit cells may also be quite difficult to visualize using two-dimensional illustrations as evident in Figure 11. Using 3D visual representations rather than 2D images can help significantly in teaching topics related to unit cells.

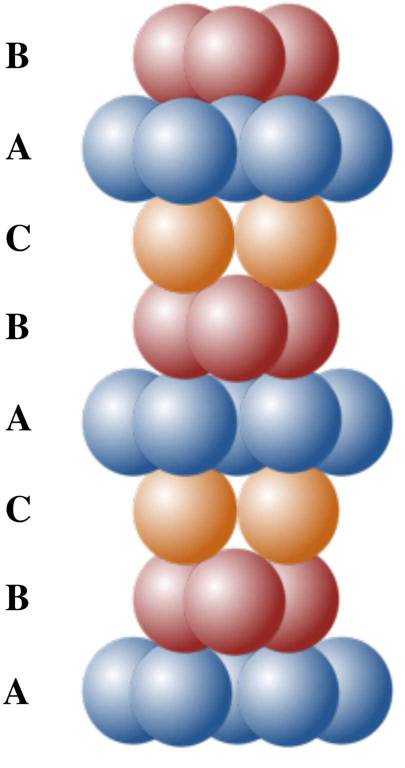


Figure 11: A standard representation of the stacking pattern in an FCC cell including the FCC close-packed stacking sequence. This image was inspired by Figure 3.31 of Fundamentals of Material Science and Engineering: An Integrated Approach, 5e, a textbook published by Wiley.[33]

Addressing Question 1 in the Design of FCC and Rock Salt Unit Cells

Many considerations were taken into account when building the FCC and rock salt unit cell models. The two models were produced with different objectives: the first to show the A-B-C stacking pattern characteristic of FCC unit cells; the other to highlight the geometric arrangement and total number of atoms in the rock salt unit cell. The designs of the FCC and one half of the rock salt unit cell models as produced in Fusion 360[12] are provided in Figure 12.

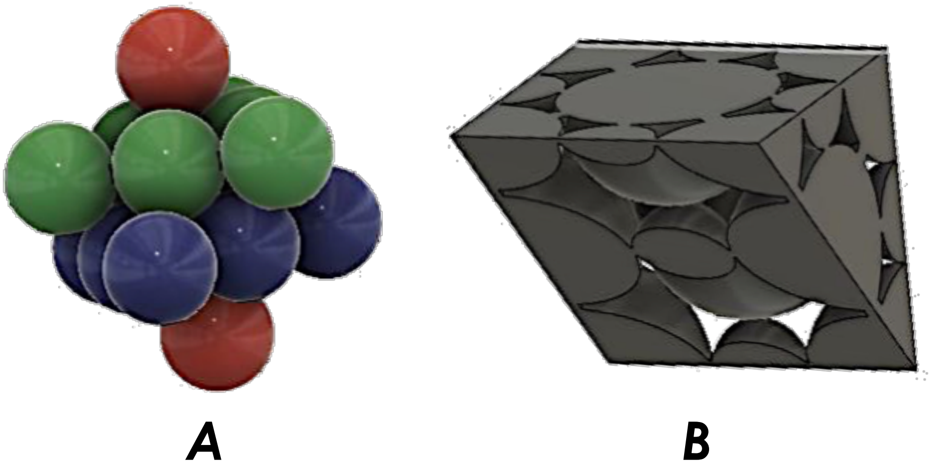
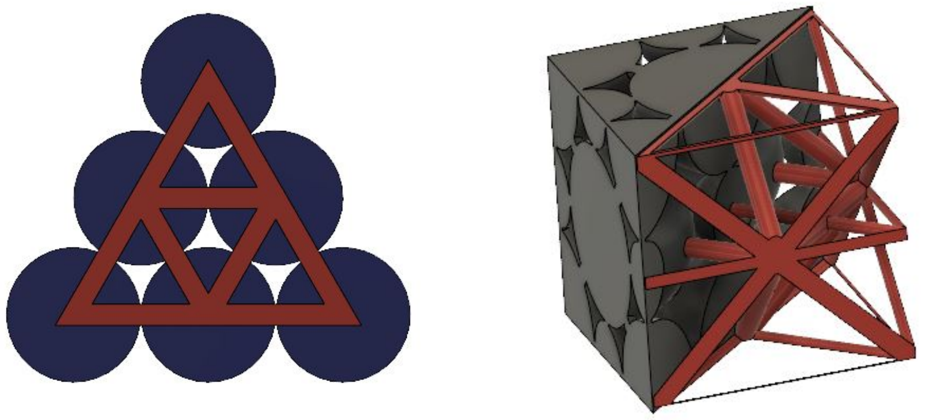


Figure 12: A) The FCC unit cell as designed in Fusion 360. B) One half of the rock salt unit cell model as designed in Fusion 360. The unit cell was cleaved across the body-center diagonal.

From an engineering standpoint, the first major challenge in creating unit cell models (and printing spheres in general) is keeping the spheres bonded to one another despite the low surface area of plastic connecting them. Especially in cases such as unit cells where no physical bonds are connecting the atoms, reinforcement of the sphere connections is vital to producing fracture resistant models. The low surface area contact between the bottom of the sphere and the print bed is also problematic

during printing and must be addressed. To decrease fragility of the models, reinforcements were introduced along the connection points between the spheres. The reinforced areas (shown in Figure 13A for the FCC model and Figure 13B for the rock salt model) were specified to print at 100% infill to produce strong, dense pockets of connecting material.



A B

Figure 13: A) The maroon areas show the reinforcement in the triangular plane of the FCC unit cell model. B) The maroon areas show the reinforcement in the rock salt unit cell model. These reinforcements are embedded in the gray spheres shown as the mirror image.

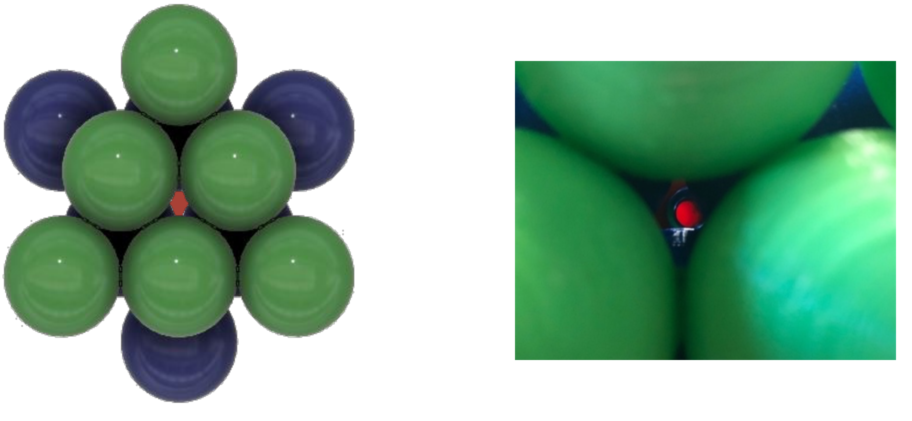
For the FCC model, to help ensure the design would print successfully, a small portion of the bottom spheres that would be in contact with the print bed was flattened to increase the contacting surface area, thereby increasing the bed adhesion and stability of the model during printing (Figure 14).

Figure 14: The bottom portion of each sphere was cleaved to increase bed adhesion and stability during printing.

Addressing Question 2 in the Design of FCC Unit Cells

The two unit cell models were designed to be taken apart and rebuilt to emphasize the main objectives of each model; the FCC model to show the A-B-C stacking pattern of FCC unit cells, and the rock salt model to highlight the number of atoms in an rock salt unit cell and their arrangement in three-dimensional space. For the FCC model, it was decided that the easiest way to show the stacking pattern was by using contrasting colors of layered spheres (Shown in Figure 12). The planes of spheres nestled precisely on top of one another to naturally create the FCC stacking pattern as depicted in Figure 12.

In addition to ease of printing and assembly, the natural alignment method used to create the FCC model also allowed for easy visualization of the interstitial spaces between atoms in the FCC unit cell (Figure 15).

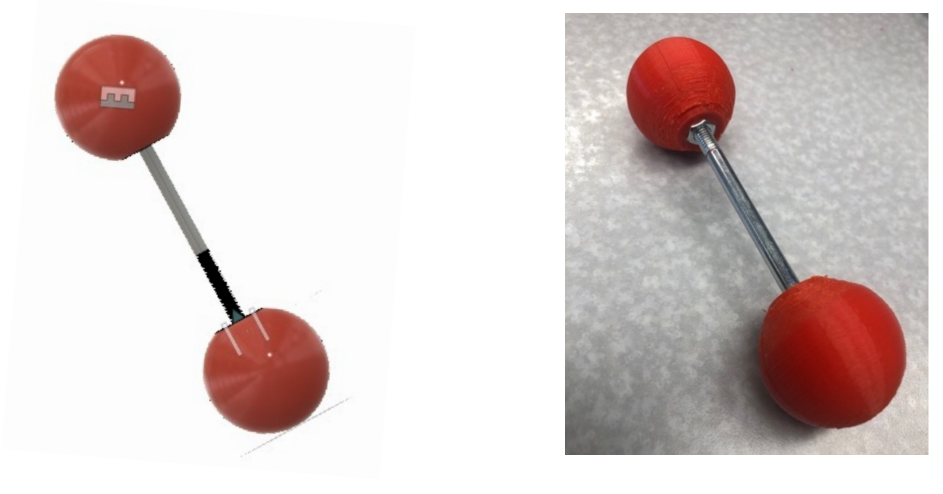


A **B**

Figure 15: A) The interstitial space can be visualized in Fusion 360 when the top red sphere is removed. B) The interstitial space is clearly visible in the physical 3D printed model as well.

For easy assembling and disassembling of the FCC model, a screw and nut mechanism was chosen. Two different pockets were added to the single end spheres of the FCC model (shown in red in Figure 16A), one for the hexagonal end of an M5 bolt long enough to reach to the opposite side of

the model, and the other to accept a hexagonal M5 nut with extra space beyond for excess length of the bolt to rest. Reinforced areas of 100% infill were added around both pockets for added strength and durability. The resulting physical screw-and-nut mechanism is shown in Figure 16B. If it is critical for the screw and nut mechanism to withstand large amount of force, consider testing the strength of the assembled mechanism first in a controlled manner.[34]



A **B**

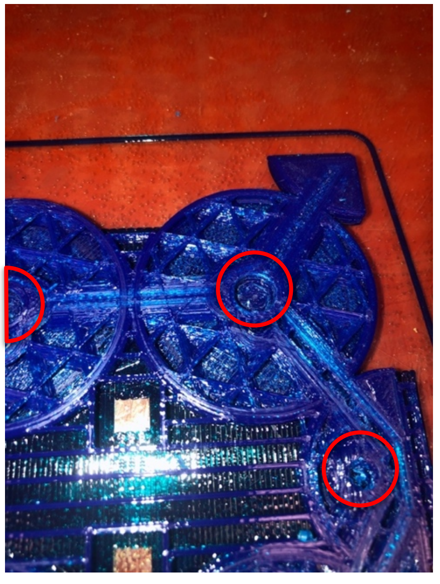
Figure 16: A) The screw and nut mechanism visualized in Fusion 360. B) The assembled physical screw and nut mechanism.

For the rock salt model, the unit cell was cleaved across the body diagonal to showcase the spatial relationship between the atoms both inside and outside of the unit cell. The eighth spheres shown in each of the eight corners of the cube and the half spheres on each of the six faces were shown rather than full spheres at each location (as present in the FCC model) to emphasize the four full-atom volume characteristic of FCC unit cells (Figure 17).

Figure 17: One half of the rock salt unit cell model. Note how the atoms were sliced to yield a perfect half-cube structure and show the eight and half spheres present in the model.

For easy assembly and disassembly of the rock salt model, a system of neodymium magnets was used. The magnets were embedded in the 3D-printed model and offered enough attractive force to hold the model together while not compromising the aesthetic of the model, nor the ability for it to be easily taken apart. The cavities for the magnets were positioned close to the body-center-diagonal face of the FCC model such that only a few millimeters of plastic would separate the magnets on one half of the model from the magnets on the opposite half. Any increase in distance between magnets was expected to significantly reduce the attractive force between them. A "pause" command was manually written into the

g-code immediately after the final layer of plastic building the magnet cavities was printed (Figure 18A), instructing the 3D-printer to stop printing until the user pressed resume on the machine. This pause allowed for insertion of the magnets into the printed cavities (Figure 18B).



A **B**

Figure 18: A) The fully printed pockets designed to hold the neodymium magnets are circled in red. B) The base of the unit cell model with magnets inserted. After resuming the print, the remainder of the model was successfully built.

Addressing Question 3 in the Design of FCC Unit Cells

Both the FCC and rock salt unit cell models were intended to be shown and manipulated as visual aids on a document camera, projected onto a large screen in a roughly 450-person capacity lecture hall environment. Several additional design strategies were employed to improve the overall efficacy of the models in this specific educational environment.

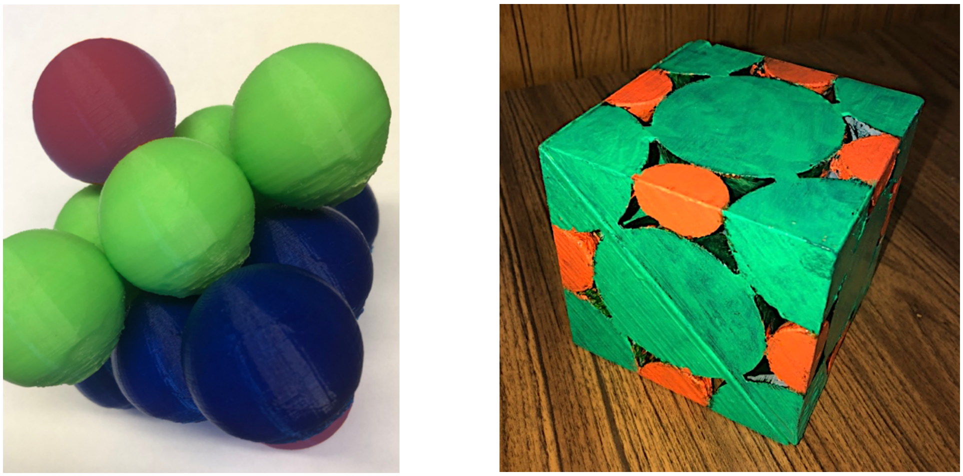
While seemingly menial compared to other design elements, color plays an essential role in comprehensibility of visual aids. Meaningful color choices

for the FCC model in particular were absolutely essential, as color was the principle attribute highlighting the A-B-C stacking pattern in the FCC unit cell. The colors chosen (purple, dark blue, and green) were not only highly contrasting, but also differentiable by sufferers of common color-blindness maladies.

Size was another essential factor in creating the FCC and rock salt unit cell models. If the model was designed too small, the print quality (especially in its spherical components) could have suffered greatly and support material may have become quite difficult to remove rendering the models produced unprofessional in appearance and ineffective in functionality. Scaling the size too high, however, could result in cumbersome models ill-suited for easy handling and an unnecessary increase in filament usage, printing time, and wear-and-tear on the 3D printer. For the purposes of this project, 1.5" sphere diameters were chosen, yielding roughly 4" cubic objects.

The final FCC and rock salt unit cell models produced after post processing (detailed in the SI) are shown below in Figures 19A and 19B, respectively.

All design files and g-codes for the models produced herein can be found in the Tutorial (see page 53 onward). While the design files were produced in Fusion 360, they are compatible with most open and close-source design software packages including FreeCAD[13].



A B

Figure 19: A) The final FCC unit cell model with screw mechanism after post-processing. B) The rock salt unit cell model after post-processing. The two halves of this model are held together by magnetic attraction.

Diagnosing and Resolving the Cause of Failed Prints

Although 3D-printing technology has become significantly more reliable and refined in the past several years, occasional failed prints are an inevitable reality of any technology. Many novices become weary of adapting 3D-printing technology for fear that when a print failure occurs, they will be unable to correct the issue. However, such fears should not dissuade individuals from pursing 3D-printing technology because upon its adoption, they will automatically join a large, supportive, knowledgeable, and collaborative virtual 3D-printing community of passionate individuals willing to offer their expertise. In fact, in addition to free public forums available for virtually all open-source 3D printers, thousands of resources including articles, YouTube videos, Facebook groups, and blog posts may be utilized to easily troubleshoot and resolve common hardware, software, and firmware issues. Discussed below is a specific issue that arose during printing of the unit cell models, how the virtual 3D printing community helped in troubleshooting the issue, the final resolution, and a general

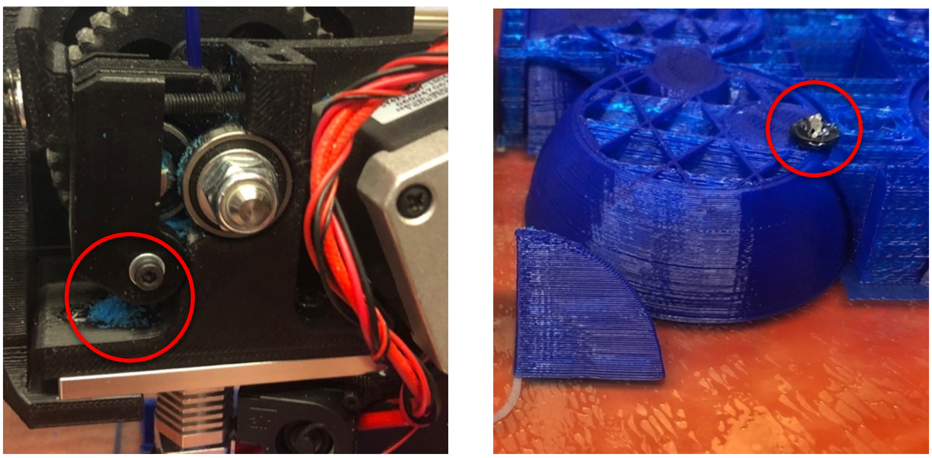
process for identifying, diagnosing, and resolving the cause of failed prints when they invariably occur.

While printing one of the unit cell models, a catastrophic print failure occurred. Pulverized filament had accumulated on and around the hot end assembly (Figure 20A), a singular mound of burnt plastic material appeared on the 3D print (Figure 20B), and mid-air "phantom" printing (the machine continuing to move as instructed by the g-code despite no filament being extruded) was noted.

Just as if diagnosing an illness, the first step taken in resolving the cause of this print failure was attempting to diagnose the issue based on its symptoms. A quick online search yielded an enormously helpful forum posted on Lulzbot's website by an individual experiencing a similar dilemma, later diagnosed as filament grinding.[35] *As evident throughout the four-page forum, several individuals in the 3D-printing community came forward to offer their hypothesis as to the cause of the issue and potential solutions.*

The information provided in the forum pointed towards three main possible causes of the filament jam: overly high tension on the filament feed-through mechanism, plastic material clogging the internal components of the hot-end assembly, or a heat creep failure. As the least invasive potential correction method, the tension applied to the filament feed-through mechanism was first loosened slightly. Shortly after, another filament jam occurred, and the hypothesis of a clogged hot-end assembly was adopted. To clear the hot-end assembly, a method referred to in the forum as a "cold pull" was explored and easily conducted with guidance from a YouTube video posted by an un-related member of the 3D-printing community.[36] *Unfortunately, the filament grinding issue persisted, pointing towards the most difficult to correct diagnosis; heat creep failure.*

Armed with this knowledge, a phone call to Lulzbot's technical support team identified the most likely cause of the issue as insufficient cooling by a sub-optimally performing heat sink fan. The fan was replaced with a higher functioning model following a fan-replacement tutorial on Lulzbot's website to ultimately resolve the issue.[37]



A **B**

Figure 20: A) The area where pulverized filament is visible is circled in red. B) A singular mound of burnt filament was formed (circled in red).

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Through the process of addressing the filament grinding print failures experienced in this work, a clear procedure for diagnosing, troubleshooting, and resolving any 3D-printing failure was ascertained:

- *Step 1: Note specific characteristics of the failed print*
- *Step 2: Research the symptoms of the print failure. Has anyone else posted about a similar issue? If so, what were the possible diagnoses? What advice was given to that individual and what methods did they use to correct the problem?*
- *Step 3: If the issue has not yet been addressed on a public forum, post the inquiry on an appropriate platform (often a forum on the printer manufacturer's website or community Facebook page). Help others work to solve the issue by including pictures, videos, the g-code file, and any other potentially useful documents in posts.*
- *Step 4: After gathering hypothesis for potential diagnoses, rank the diagnoses in order of increasing invasiveness of the related corrective measures.*
- *Step 5: Begin implementing potential solutions or countermeasures. Assume the most easily treatable diagnosis is in fact the issue and employ the respective corrective measure. If the issue persists, dismiss the hypothesized diagnosis and move on to the next least-invasive corrective action until the issue has been properly diagnosed and resolved.*
- *Step 6: If the dilemma was posted on an online platform, continue actively posting in the discussion. Noting whether or not each proposed*

corrective measure solved or reduced the problem can not only help to correct the issue, but also advances knowledge in the 3D printing community and may benefit someone else with a similar issue in the future.

As knowledge of 3D-printing and experience in resolving issues is gained, consider following forums and helping other beginners to further advance growth in the 3D printing community.

Future Works

In the future, the use of several different thermoplastic materials will be explored including analysis of the advantages and disadvantages of each material and potential applications. The use of thermoplastic elastomers (TPE) for example, would yield flexible molecular models allowing for bending, twisting, and stretching of molecular bonds. The elasticity of the model could prove very effective in showing the common vibrational modes present in a molecule including rotational and stretching bond movement among other uses, however, may present unique challenges as it is a more difficult material to print with than PLA or ABS.

Another area of interest which could benefit greatly from further inquiry are applications of 3D-printed models and visual representations for different age groups extended to multiple disciplines including mathematics, biological and earth sciences, technology, and engineering. 3D-printed molecular sets for an entire classroom (as opposed to the singular models produced in this work) will be studied and quantitative analyses will be performed to determine the effectiveness of 3D-printed models on academic performance.

Conclusions

This work provides a novel stepwise procedure in 3D-printing pin-and-hole style molecular structures, emphasizes the value of using 3D-printed models as visual representations in advanced topics, and outlines helpful processes for implementing design-enhancing techniques and troubleshooting the cause of failed prints. Using the proposed methods, 3D-printed models of a polycarbonate fragment structure, FCC and rock salt unit cells, and a vector model of the atom were successfully manufactured and used during a poster presentation and in college classroom environments. In fact, through the proposed procedure for producing 3D-printed pin-and-hole style molecular models, molecular sets could easily be created for entire classrooms and the components necessary to form large, interchangeable polymeric structures could be obtained much more cost efficiently.

For educators or researchers who may not have the time or resources necessary to dedicate to a 3D-printer and other required materials, there are several ways to obtain 3D-prints with similar customizability options without owning a machine. The least expensive option is looking within a university or school for a 3D-printer. Makerspaces and some libraries may also provide access to 3D-printers. If no local options are available, there are a handful of printing services that can print out single models at reasonable prizes. Some services may offer multiple color prints so each atom in the 3D-printed model follows a color code as well.

An original beneficial aspect of this work is the adherence to the open-source philosophy. Using software and firmware in which all programs and their source codes are freely available and the blueprints for hardware components fully accessible provides users with the option for complete customizability of both the model design and manufacturing process. The emphasis in the open-source philosophy on sharing collective knowledge may be well attributed to the rapid advancement of 3D-printing technology and is predicted to be a powerful force in initiating a fourth industrial revolution of innovation and technology. For this reason, the authors have decided to contribute to the wealth of designs and

information produced by members of the open-source community by making design files for all created models publicly available at:

[*https://drive.google.com/drive/folders/16b8ZPnLOJ_dz18NlCOyajGN2U4CVblgx?usp=sharing*](https://drive.google.com/drive/folders/16b8ZPnLOJ_dz18NlCOyajGN2U4CVblgx?usp=sharing)

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Tutorial for Designing Pin-and-Hole-style Molecular Models

Part 1: Creation and Exportation of the Virtual Molecular Model

In this work, virtual molecular models were built using the Gaussview 6 interface (Figure 1). The Gaussian 16 software package[1] is not open-source or freely available for non-commercial use, however any software program capable of producing molecular structures and exporting them as a program database format file (file extension .pdb) may be used. Free options for creating virtual molecular models include: Moldraw,[2] Avogadro,[3] Vesta,[4] Molekel,[5] Gabedit,[6] Jmol,[7] and Molden.[8] Virtual molecular model (.pdb) files may also be retrieved from online sources including the Cambridge Crystallographic Data Center (CCDC).[9,10]

Part 2: Using Chimera

Chimera is used to convert the .pdb virtual molecular model file into an extensible 3D (.x3d) file format. Although superseded by the .x3d file format, the Virtual Reality Modeling Language (.wrl) file format may also be used.

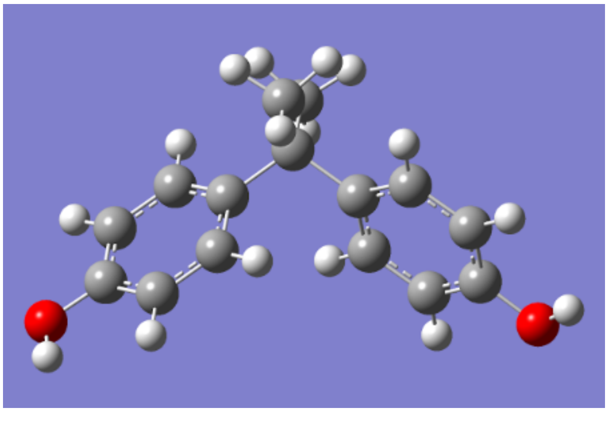

Figure 1: Molecular model created using the Gaussian16 graphical interface.

After installation of Chimera,[11] the .pdb virtual molecular model file can be opened. As shown in Figure 2, the default setting in Chimera is a "stick"-type structure as opposed to the "ball-and-stick"-type structure usually more desired for molecular models.

In addition, several bonds throughout the molecule appear split such that one-half of the bond is the same color as the atom to which it is bonded, and the other half of the bond is the color of the second atom participating in the bond. The latter will present serious challenges when attempting to split the model in Blender, as each half-bond is recognized as its own entity and manually joining each atom and bond can quickly become a grotesquely tedious task (especially for large molecules). Fortunately, both issues can easily be resolved using the "Command Line" under the "Favorites" tab in Chimera.

In the command line, the following lines of code should be pasted:[12]

```
represent b+s
~disp solvent
setattr M ballScale 0.3
setattr M stickScale 1.35
bondcolor grey
setattr p drawMode 1
vdwdefine 1.78 @o=
vdwdefine 1.8 @n=
vdwdefine 2.0 @c=
```

The resulting virtual ball-and-stick molecular model is shown in Figure 3. Note how all bonds throughout the structure are consistent in color, allowing for the bonds to be mapped as a single object in Blender[13] later on.

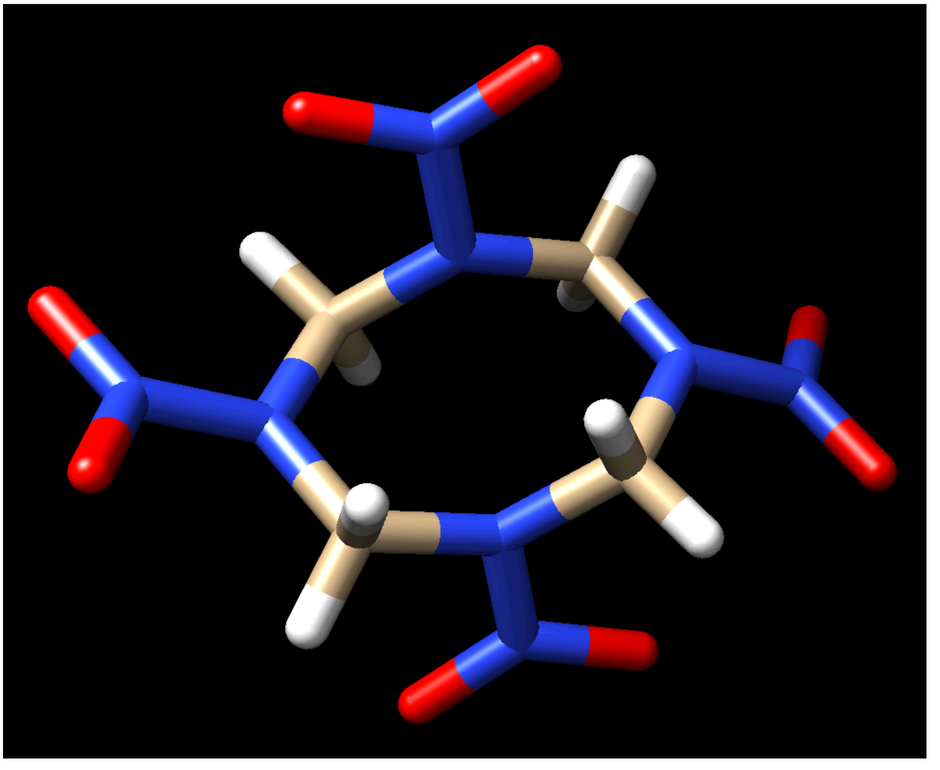

Figure 2: Virtual molecular model in Chimera prior to changing default settings.

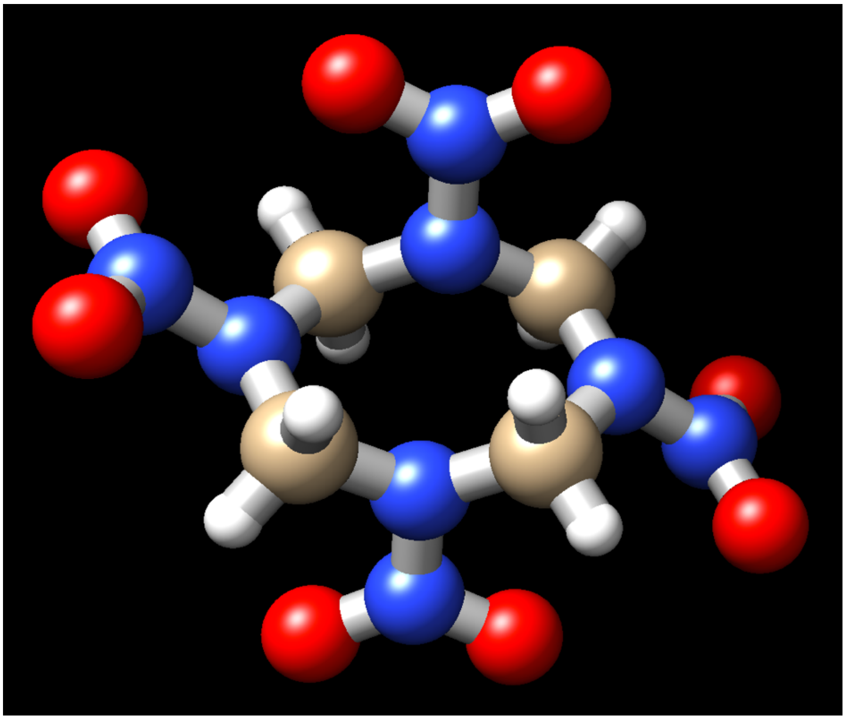

Figure 3: Virtual molecular model in Chimera after imposing the lines of code outlined above in the "Command Line".

The virtual molecular model may now be exported as a .wrl or .x3d file format for processing in Blender. If the molecule does not need to be split into components, export the file as a Stereolithography (.stl) file format.

Part 3: Blender and the MolPrint3D add-on

The MolPrint3D[14] add-on for Blender is used to split the molecular model into components and allows for the creation of pins and holes throughout the model. Unless the molecular model surpasses the volume of the print bed, it is not technically necessary to split the model into components, however a well-thought-out splitting plan may significantly decrease the amount of support material needed thereby reducing the print time and material usage.

While certainly not difficult, as an add-on, the installation of MolPrint3D is slightly more intensive than the other software programs utilized. A complete instructional video for the installation of MolPrint3D has been provided by the developer.[15] In this work, the most recent releases of both Blender and MolPrint3D were installed.

Upon first opening the Blender software, several default objects will appear (Figure 4).

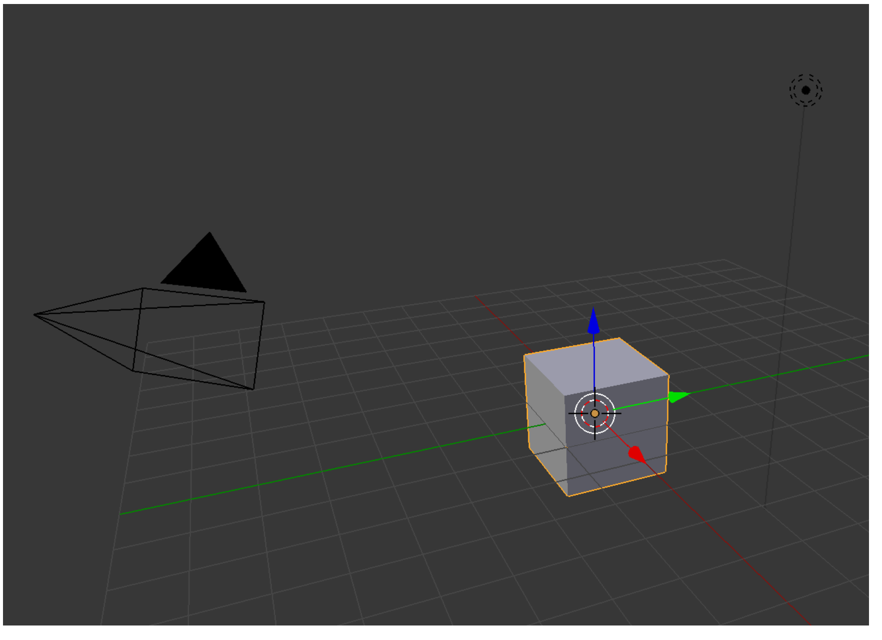

Figure 4: Default objects in Blender on start-up.

To delete these objects, press the "a" key twice, followed by the "x" key, and finally the "enter" key. Using the "Import VRML" button in the MolPrint3D add-on tab, import the .wrl or .x3d file created in Chimera. The "primitiv" factor changes the resolution of the spheres. As shown in Figures 5 and 6, a low value for "primitiv" results in a pixelated-like surface and a high value produces a smoother, more spherical appearance.

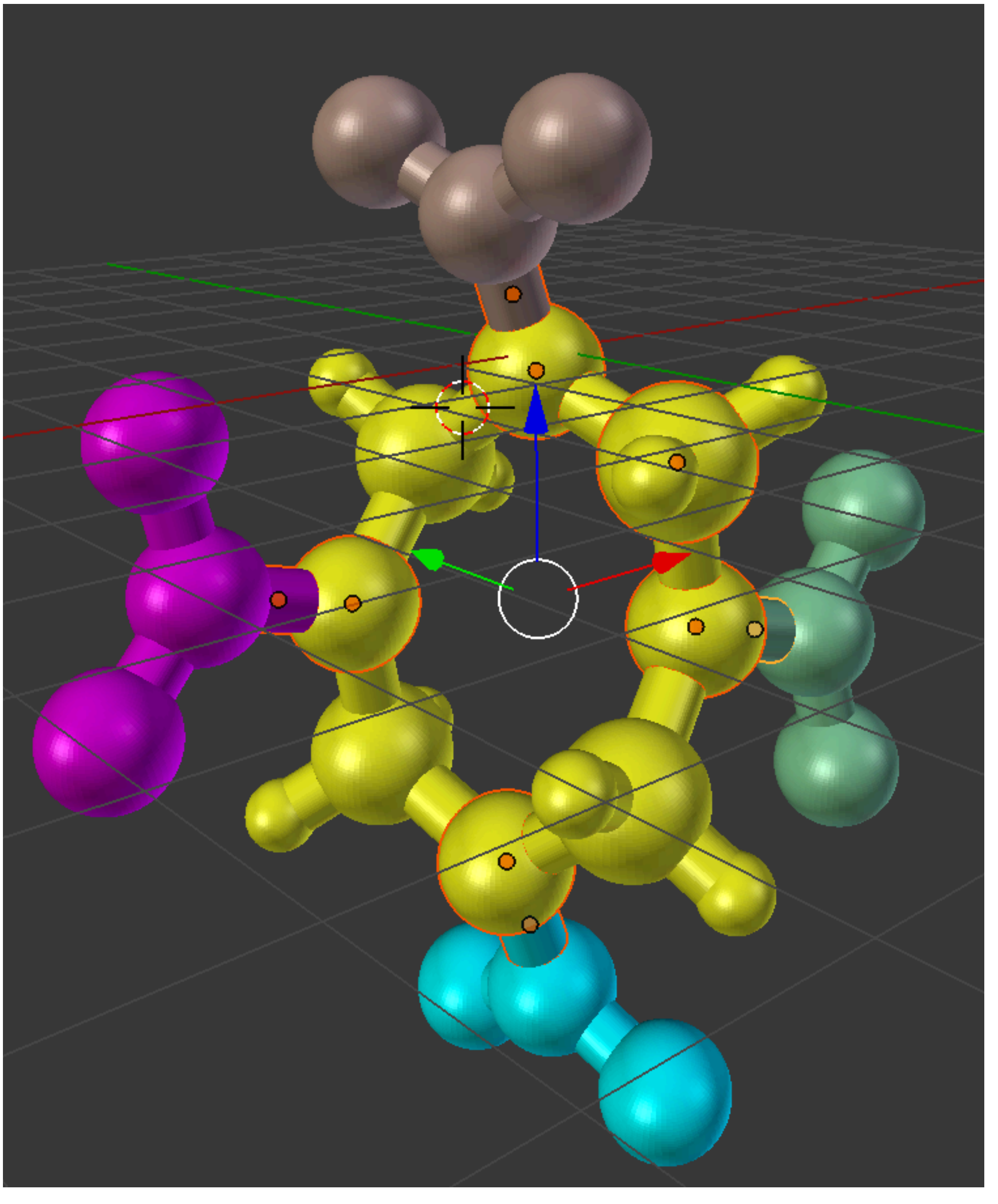

Figure 9: This molecule has been split into five components, each of which are relatively planar.

There were two primary methods for producing connecting pins used in this work, one in which one side of the connecting bond has a pin to connect to an adjacent atom (method 1), and the other in which both sides of the bond have a connecting pin and the bond is printed as a separate entity

(method 2). Method 1 (shown in Figure 10) is ideal for most situations, however method 2 (Figure 11) may be more appropriate in some cases.

For example, when printing molecular models containing stacked ring structures (as in Figure 12), method 1 may not be capable of separating the model into semi-planar components as efficiently as method 2.

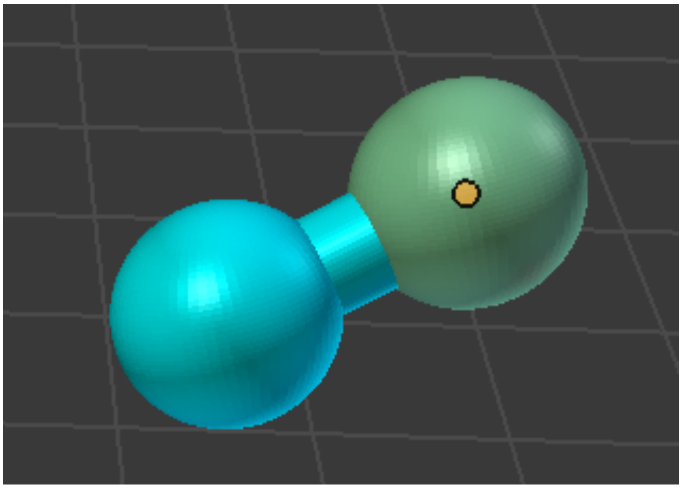

Figure 10: Method 1 for producing pin-and-hole mechanism. The bond is attached to one atom.

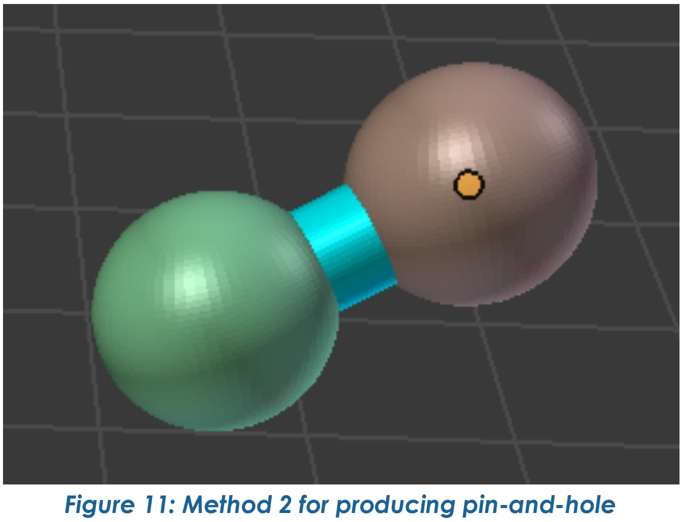

Figure 11: Method 2 for producing pin-and-hole mechanism. The bond is independent of both atoms.

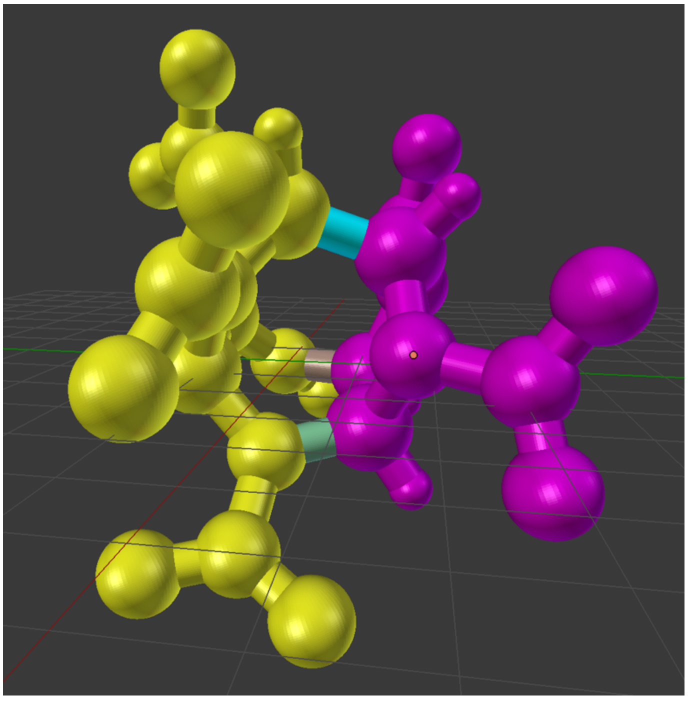

Figure 12: Separation of a molecular model containing stacked ring structures using Method 2.

To separate model groups via method 1, select the area where the pin-and-hole mechanism should reside by right-clicking on a single bond and adjoining atom while holding the "shift" key. To separate model groups via method 2, select a bond to be printed as a separate entity by right clicking on the bond and both attached atoms. It is important to note there are many other ways to select components, however methods 1 and 2 were found to be the most convenient options, applicable to many cases. Creating atom groups may appear tricky at first, but with a bit of practice, it becomes a very quick process.

After the molecule has been grouped into its desired components, use the Pinning/Joining feature to produce the pin-and-hole mechanisms. The pin side designates the number of faces, and therefore the geometric area, the pin will have. For example, a Pin side of 4 will produce a square-shaped pin, while a pin side of 6 will produce a hexagonal-shaped pin (Figures 13 and 14, respectively). The minimum number of pin sides possible is 3,

producing an equilateral triangle and resulting in the least number of possible conformations once the model is printed. Conversely, a high number of pin sides will produce a round pin capable of achieving 360° rotation.

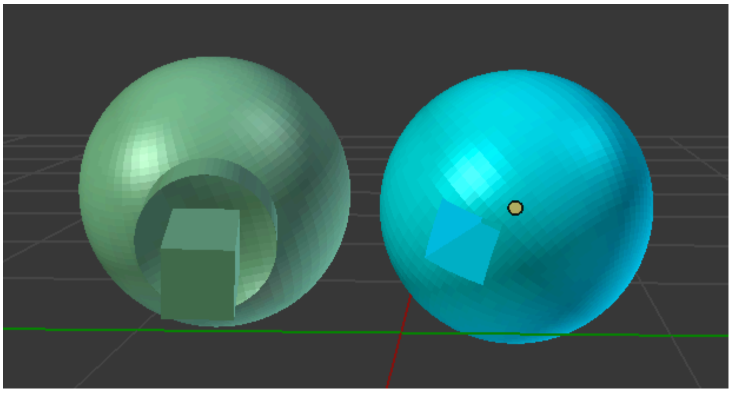

Figure 13: Choosing a pin side number of four results in square-shaped pins and holes.

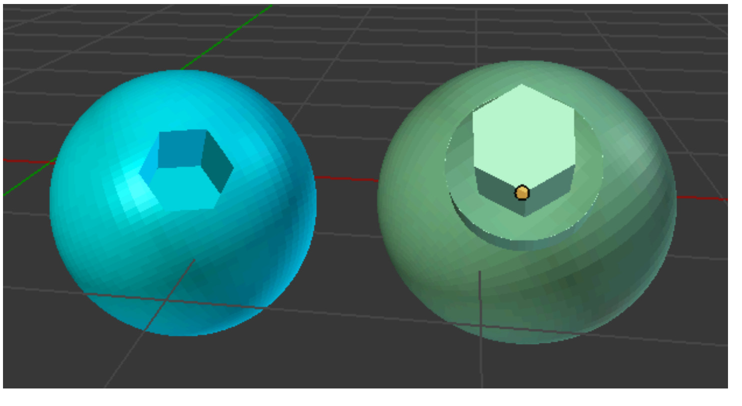

Figure 14: Choosing a pin side number of six results in hexagonal-shaped pins and holes.

The pin bond and hole size can be used to adjust the tolerance between the pin and hole. It is imperative that experimentation be conducted prior to printing a large molecular model to appropriately adjust the pin and hole

size. A simple, low-waste method for choosing the pin and hole sizes is addressed in Part 6: Pin-and-hole Size Experimentation.

After adjusting the number of pin sides, pin size, and hole size, create the pin-and-hole mechanism my clicking "Set Pin Group" followed by "Pin and Join". Ensure the pin-and-hole mechanisms are correctly formed by right clicking on the different components and moving them to visualize the pins and holes created. Two common issues apparent upon visualization are circled in Figures 15 and 16. If such issues appear continuously, try importing the .wrl or .x3d file at a lower resolution (primitiv number) or if a .wrl file format was used, try using an .x3d file instead (and vice-versa). It may also be necessary to choose a different location for the pin and hole.

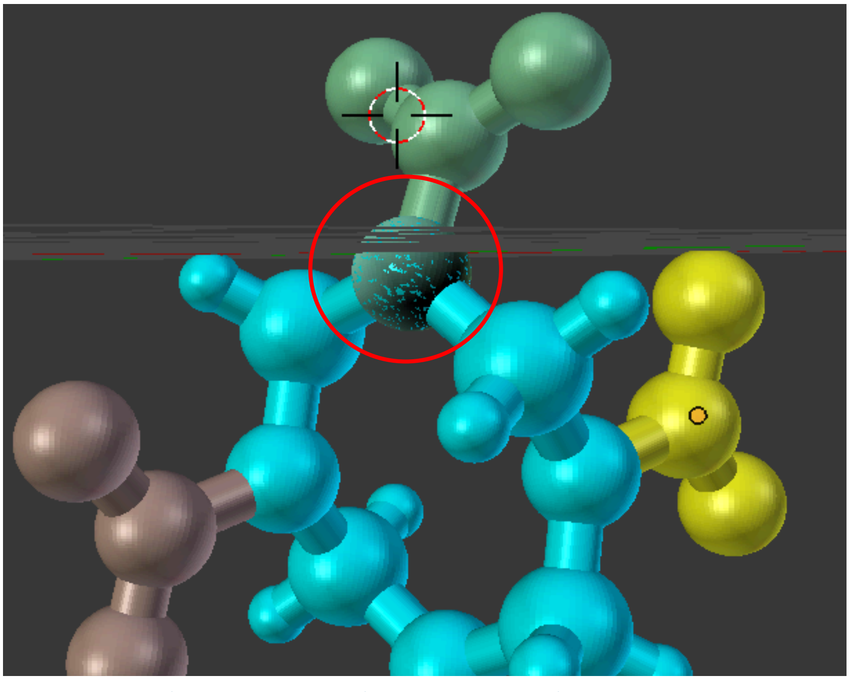

Figure 15: In the circled area, no pin-and-hole mechanism was formed.

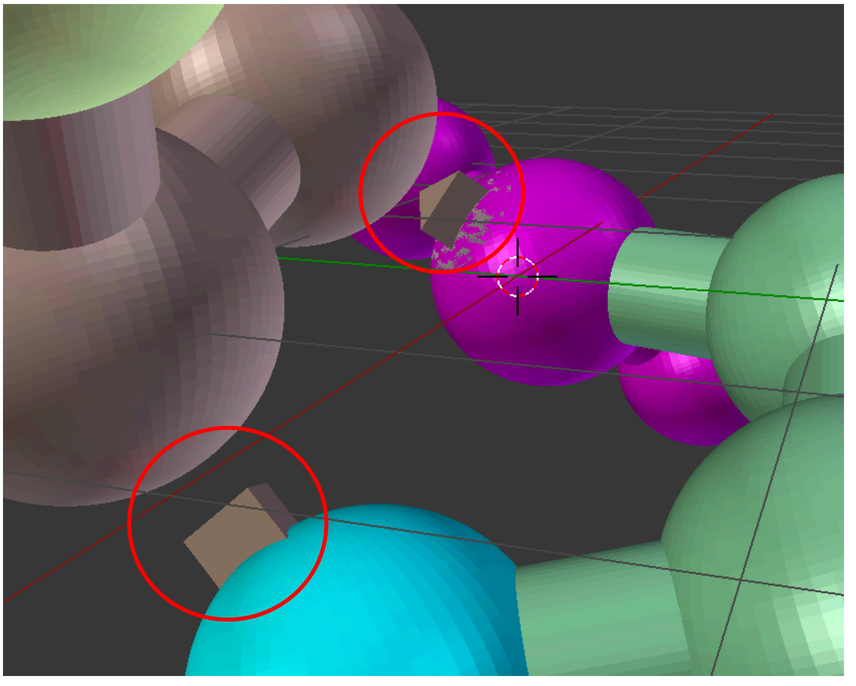

Figure 16: In the circled areas, the pin-and-hole mechanisms were formed incorrectly.

Once the pins and holes have been successfully created, the molecular model should be exported in a .stl file format. It is not recommended to use the "Floor and Export" feature in MolPrint3D. Each time the author attempted to use the floor and export feature, Blender would quit unexpectedly (at least when using the Mac iOS operating system) and all work up to that point was lost if not previously saved. Furthermore, using the methods described herein, "flooring" (aligning the components most flatly on the print bed) is conducted later on in the final stages of g-code preparation. Further information and tutorials for the use of Chimera, Blender, and MolPrint3D have been produced by the developer of MolPrint3D as a series of helpful YouTube videos.[16]

Part 4: Scaling and Splitting

To obtain the best possible alignment of molecular model components on the print bed, the components must be split from one another and exported as individual .stl files. Slic3r Prusa Edition[17] *V1.7.5 (not to be confused with the more recently released software package, PrusaSlicer) was found to be a convenient program for splitting components into individual files.*

After importing the .stl file produced in Part 3, the components of the molecular model will appear quite tiny as a result of length unit discrepancies between Blender and Slic3r Prusa Edition. To compensate for unit discrepancies, the model must be scaled anywhere between 2000-4000% depending on the program used to create the molecular model and user preference. Experimentation (described in Part 6) should be conducted prior to printing to determine what scaling factor produces the desired size spheres for the molecular model. Once scaled, left-click the "split" button to designate each component as a separate entity and save each component as an individual .stl file.

Part 5: Preparation of the Final g-code File

For preparation of the final 3D-printable g-code file, it is recommended to use the slicer software developed specifically for the machine used if available. For example, if a 3D-printer manufactured by Lulzbot was used (as it was in this work), Cura Lulzbot Edition[18] *should be used to prepare the final g-code. Likewise, if a 3D-printer manufactured by Prusa was used, PrusaSlicer*[17] *would be the appropriate slicer to use for building the final g-code file.*

Regardless of the slicer software package used, it is vital to properly align the models on the print bed, enable the addition of support material, and choose the proper temperature settings for the filament used if applicable. Components of the molecule should be aligned as flat as possible on the print bed to reduce the amount of support material needed and holes for

the pin-and-hole mechanism should be positioned on top of the model rather than on the bottom to prevent material from filling in the hole. For most prints, if it is not feasible to position holes on the top of the model, excess material in the holes is usually fairly easy to remove using a pair of tweezers and flush cutters. Proper alignment of a molecular model component is illustrated in Figures 17 and 18.

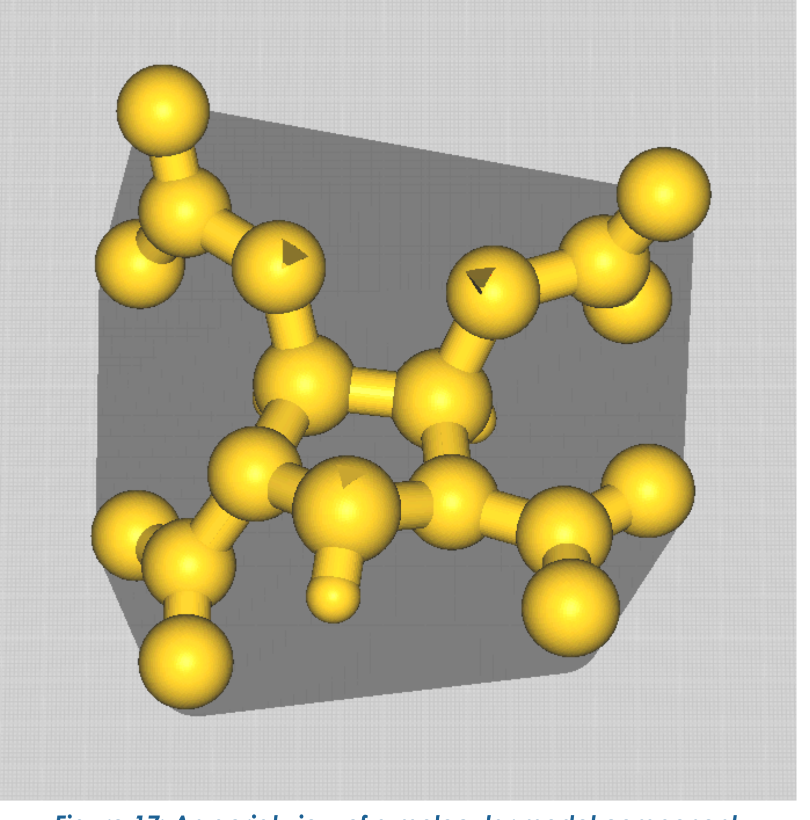

Figure 17: An aerial view of a molecular model component in Cura Lulzbot Edition. Note how the holes of the pin-and-hole mechanism are positioned on top of the model.

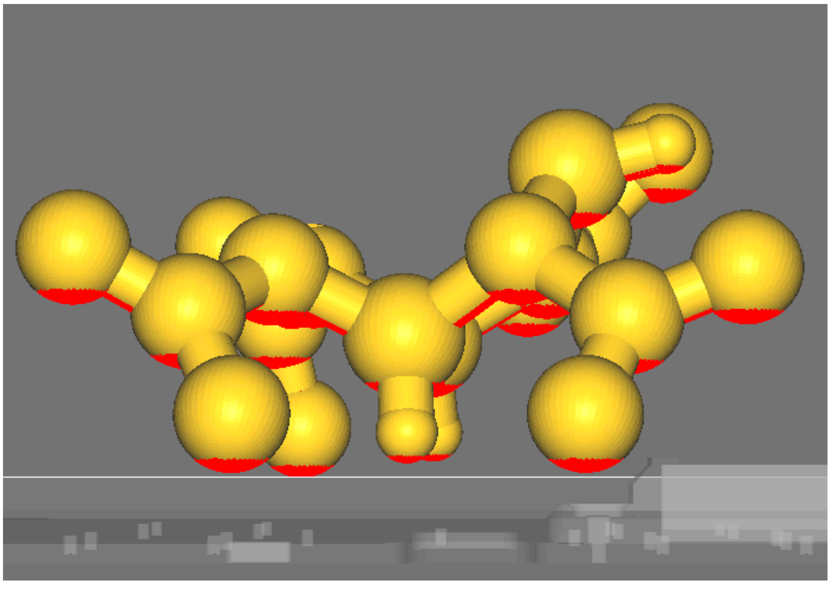

Figure 18: A side view of a molecular model component in Cura Lulzbot Edition. As shown, the component is positioned as flatly as possible on the virtual print bed.

The use of support material is very important when printing molecular models. Printing spheres using FDM-style 3D-printers is inherently difficult due to the low contact surface area characteristic of spherical geometries. Without the use of support material to hold the spheres in place by increasing the number of contact points between the sphere and surrounding material, the print is all but guaranteed to fail due to instability and improper adhesion. Many slicers including Cura Lulzbot Edition and PrusaSlicer have support-generation features which automatically build adequate support structures when enabled. A molecular component with support material generated in Cura Lulzbot Edition is shown in Figures 19 and 20.

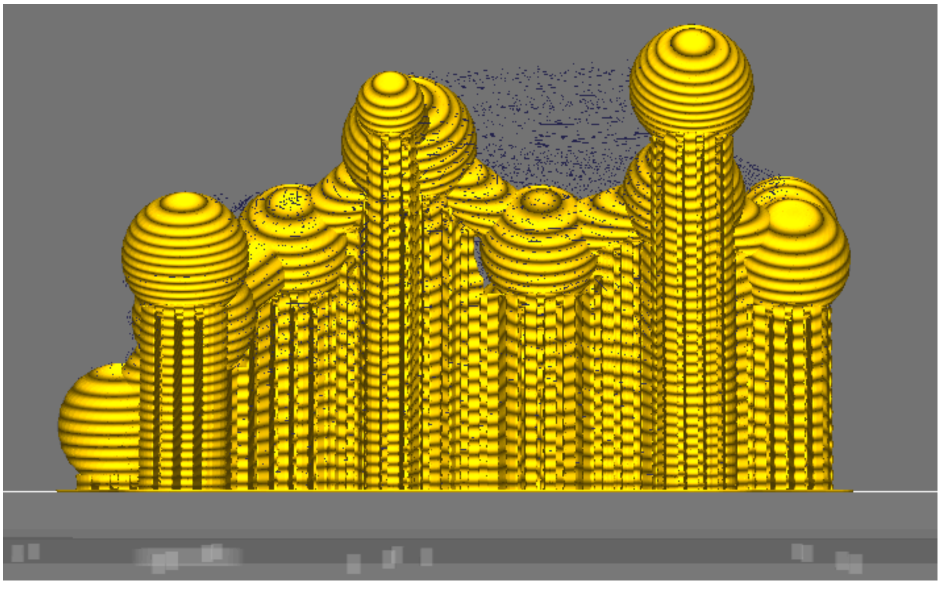

Figure 19: Side view of a molecular model component with added support material.

After the models have been properly aligned, correct temperature settings applied, and support material generated, the molecular model components may be exported as a g-code (.gcode extension) file. The .gcode file can be transferred to an SD card (for most FDM-style 3D-printers) and used to print the physical 3D-printed molecular models.

Part 6: Pin-and-Hole Size Experimentation

Several factors including the scaling factor used in Slic3r Prusa Edition, the size of the extruder, slight variations unique to the exact 3D-printer used, and personal preference of the user will affect the pin and hole sizes necessary to achieve the desired tolerance. Each printer will likely require different settings for the pin-and-hole sizes to produce an acceptable tolerance level, and for this reason, it is necessary to experiment with pin-and-hole sizes.

Waste reduction is an important consideration when experimenting with pin-and-hole sizes. To reduce waste, it is recommended to only print one or

two atoms and a single bond connected through a pin-and-hole mechanism within one of the molecular model components rather than experimenting on entire components of the molecular model. As the original size of the molecular model may vary depending on the program used to create the .pdb file and the scaling factor imposed in Slic3r Prusa Edition, it is recommended to isolate an atom and bond within the molecular model to be printed and impose a pin-and-hole mechanism to test the tolerance level. To change the size of the pins and holes, change the pin bond and hole size options in Blender prior to imposing pins as discussed in Part 3: Blender and the MolPrint3D Add-on. Only make conservative changes when adjusting pin and hole sizes, as a relatively small change in the value can make an incredibly large difference in the pin or hole size. This process if further illustrated in Figures 21, 22, and 23.

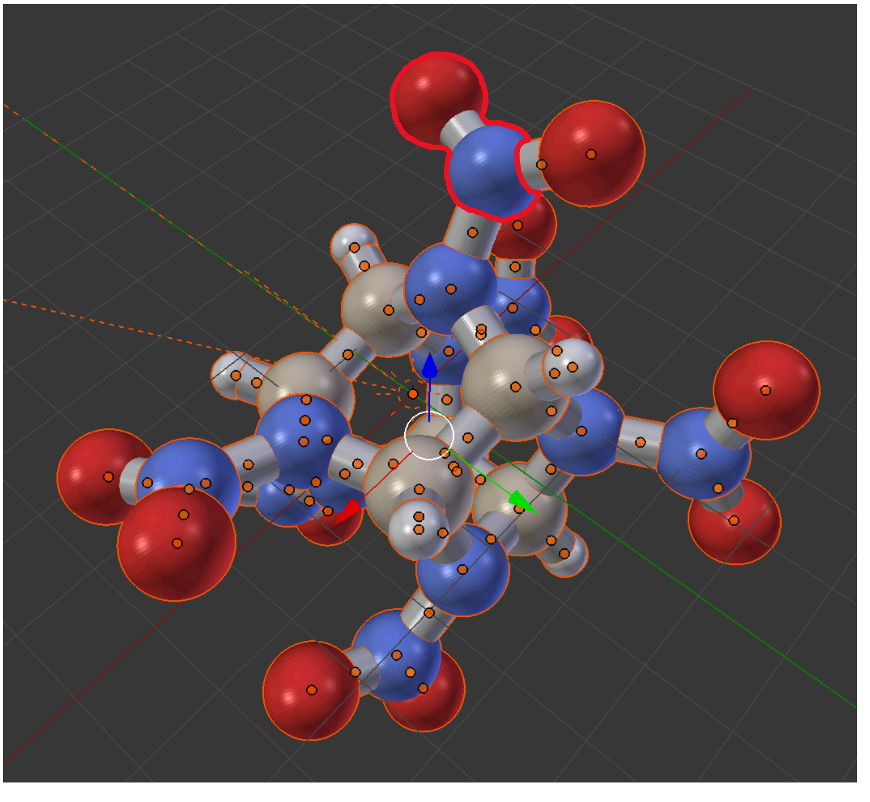

Figure 21: All atoms and bonds within the molecular model were selected and deleted in Blender, isolating only the two atoms and connecting bond circled in red.

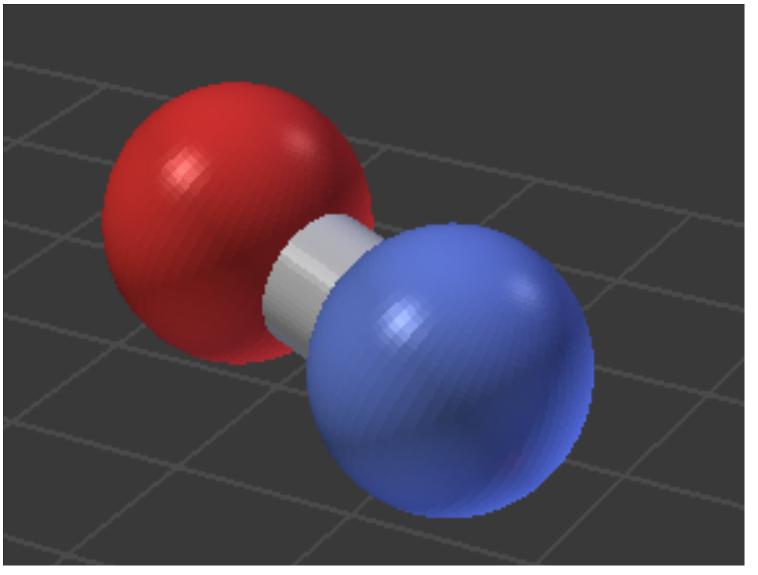

Figure 22: The two atoms and bond isolated from the molecular model shown in Figure 21

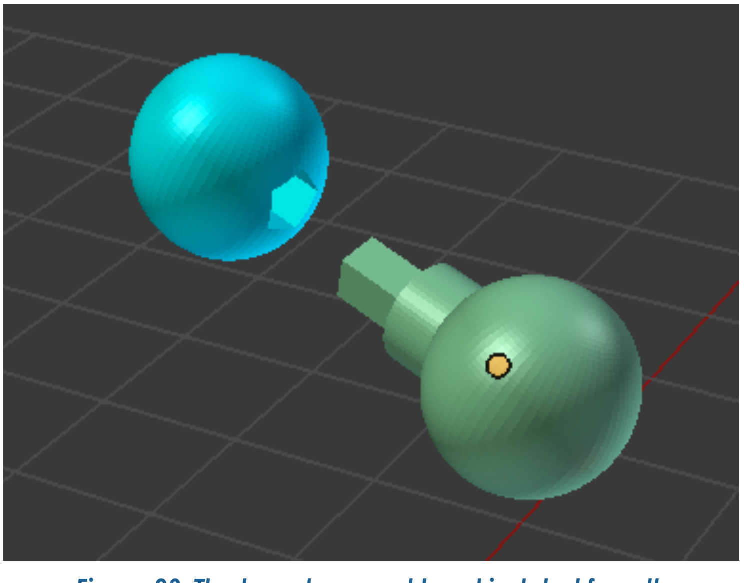

Figure 23: The two atoms and bond isolated from the molecular model shown in Figure 21 with the pin-and-hole feature enabled via the methods discussed in Part 3: Blender and the MolPrint3D Add-on.

In addition to testing the pin-and-hole tolerance, performing test prints also provides a physical indication of how big the final molecular model will be. If the printed sphere appears too small, the components should be scaled up in size slightly in Slic3r Prusa Edition, and conversely, if the printed sphere appears too large, the components should be scaled down slightly. Because the pin-and-hole size is contingent on the scaling factor, the scaling factor should be chosen prior to adjusting the pin-and-hole tolerance.

Post-Processing Methods

As emphasized several times herein, one of the major advantages of 3D-printing molecular models is the potential for full customizability. Post-processing of the 3D-printed models offers an entire new branch of customization possibilities beyond differentiation in design features. In addition, post-processing is essential to the overall functionality and effectiveness of 3D-printed objects, especially in the case of educational models. A detailed account of the post-processing methods used, including both failures and successes is explored below.

Filling, Sanding, and Painting

With proper filling, sanding, and painting technique, 3D-printed molecular models can be made to look as if they were injection-molded in a factory using costly, high-tech equipment.

Filling can be accomplished using a "filler-primer" paint or spray paint. This special type of paint contains course particles which are able to "fill in" any crevices or divets present on the surface on an object, including the characteristic layer lines of 3D-printed objects.

After the filler-primer paint is applied and allowed to dry completely, the 3D-printed object should be sanded for a smoother finish. Multiple coats of filler-primer paint may be applied if needed according to the directions on the product. A unit cell model before and after filling and sanding is shown in Figures 24 and 25, respectively.

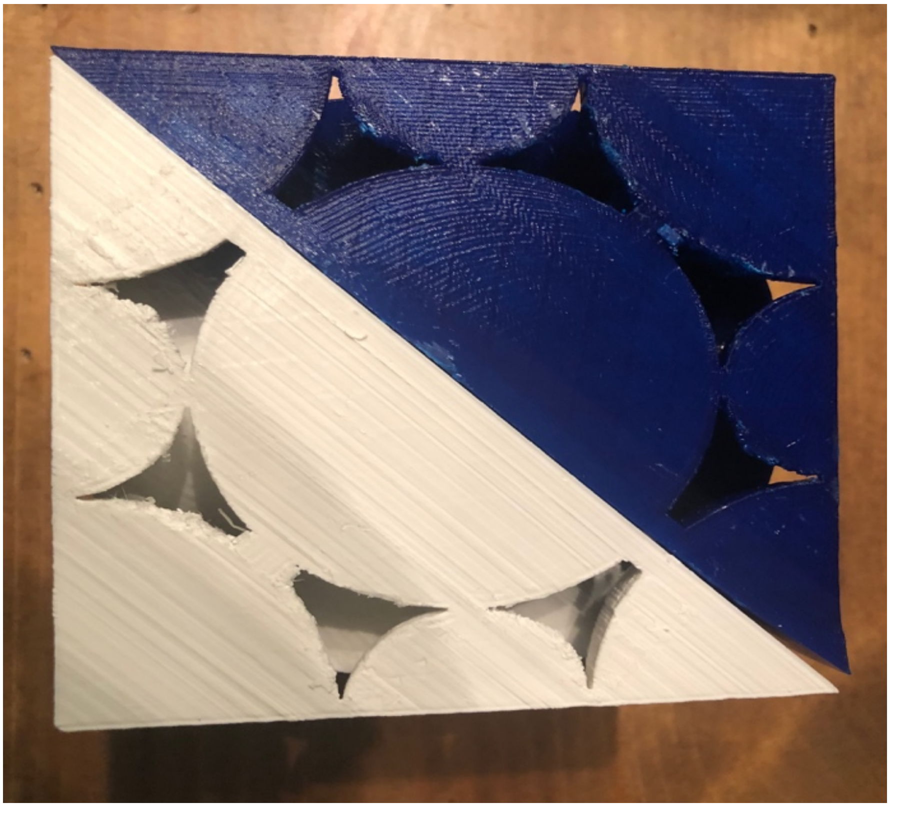

Figure 24: 3D-printed object prior to coating with filler-primer paint and sanding.

Figure 25: 3D-printed object after coating with several layers of filler-primer paint and sanding. Note the reduction in appearance of layer lines throughout the object.

Painting can be done with or without first painting and priming the 3D-printed object. In this work, acrylic paint was used to paint the model. If a glossy finished is desired, the model may also be coated with a clear-gloss finish after painting. When painting molecular models, it is advisable to use standard color conventions (i.e. white for hydrogen atoms, red for oxygen atoms, blue for nitrogen atoms, etc.), as shown in Figure 26. If printing models without standardized color conventions, consider choosing color-blindness-friendly color schemes such as orange, green, and purple, especially if the model will be used in classroom environments with many students.

As an important safety consideration, always read directions and warnings when using non-familiar paint products. In addition, paints should only be used in well-ventilated areas, as many paint products may produce irritating or dangerous fumes.

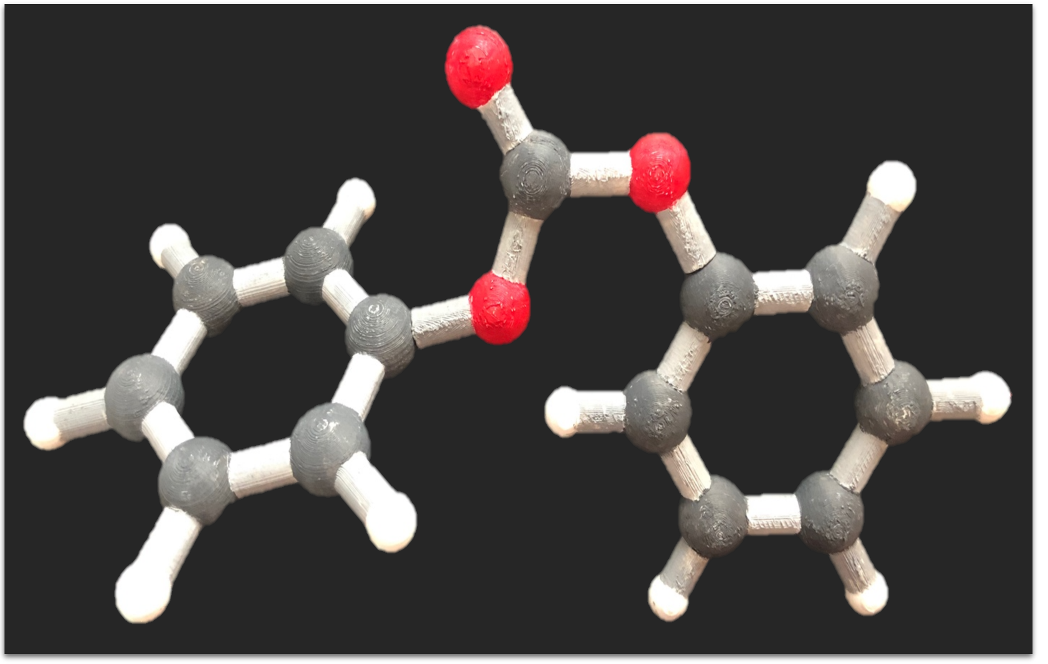

Figure 26: A molecular model painted using a conventional color scheme: red denoting oxygen atoms, gray for carbon atoms, and white for hydrogen atoms.

Acetone Smoothing for ABS

A very useful feature of specifically ABS thermoplastic material is its ability to dissolve in acetone. Using acetone smoothing techniques, the layer lines of objects 3D-printed in ABS material may easily be removed without the use of filler and primer products.

Many creators and 3D-printing hobbyists have developed simple methods for acetone smoothing and shared their techniques on community forums.[20-22]

As shown in Figures 27 and 28, acetone smoothing allows for an extremely smooth, shiny finish with much less effort than repeated application of filler-primer paint and sanding.

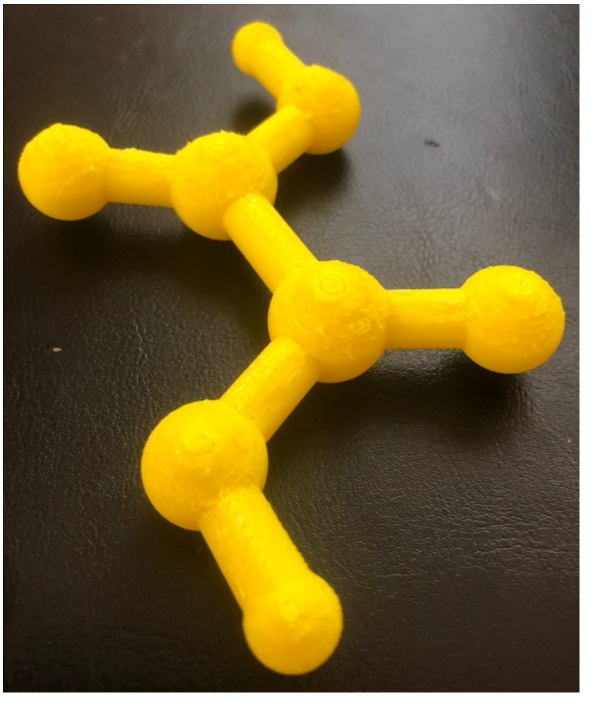

Figure 27: An ABS 3D-printed molecular model before acetone smoothing. Note the roughness of the bottom of the spheres after removing support material.

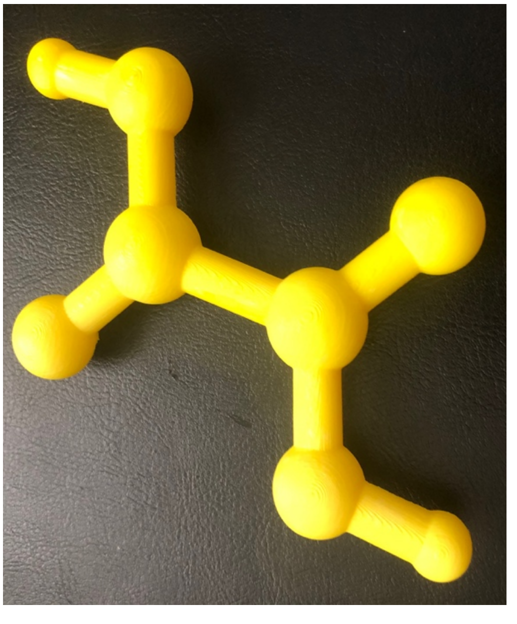

Figure 28: An ABD 3D-printed molecular model after acetone smoothing. Not how the bottom of the spheres where support material was removed is now smooth in appearance.

Adding Metal Components

Introduction of metal components in 3D-printed objects may be necessary for proper functionality and increased strength. Arguably the most successful method for including metal components in 3D-printed objects is embedding the metal within the plastic material. To do so, a pocket should be designed within the 3D-object to house the metal component. A pause command can be introduced into the g-code file to instruct the printer to pause once the pocket has been printed, allowing for insertion of the metal piece. The print can then be resumed to fully embed the metal object in plastic.

If embedding the metal object in the 3D-printed component is not possible or if the metal object must protrude from the plastic part, heat-setting may successfully join the metal and plastic material for some applications. To embed an object in a 3D-printed part using heat-setting methods, carefully heat the metal object in a direct flame until it reaches a temperature greater than the melting point of the plastic material used. With firm pressure and using proper personal protective equipment, the hot metal can be pushed into the plastic resulting in a tight-tolerance fit. The nut and bolt-head in the screw and nut mechanism pictured in Figure 29 were joined to the plastic sphere using heat-setting methods.

Despite the tight-tolerance fit between the two objects, the metal component separated from the plastic under normal use conditions. To correct the issue, a special metal to plastic bonding epoxy agent was used.

Adhesives including epoxy, glues, and other bonding agents may be used to bond metal and plastic components, however for successful adhesion, bonding agents specifically formulated to bond metal and plastic should be used.

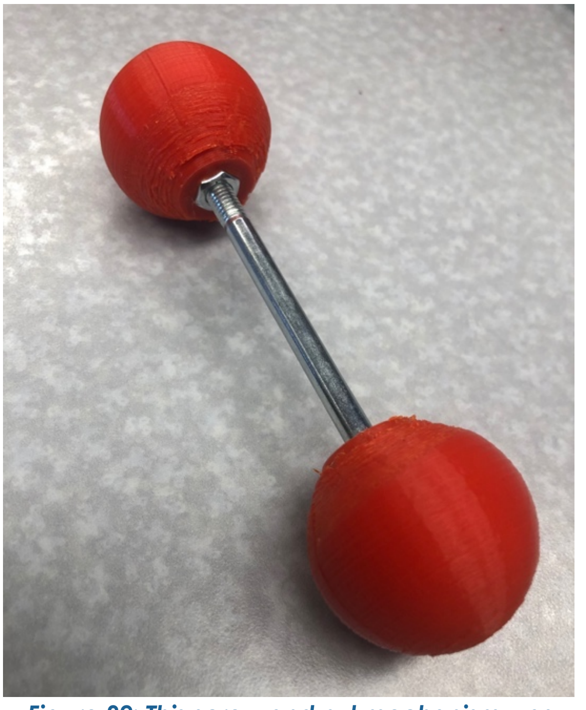

Figure 29: This screw and nut mechanism was assembled by heat-setting the nut and bolt into the plastic sphere.

Design Files

The design files for the three primary models created through this work (a polycarbonate fragment molecular model, the vector model of the atom, and unit cell models) are available in an .stl format online at the following URL:

https://drive.google.com/drive/folders/16b8ZPnLOJ_dz18NlCOyajGN2U4CVblgx?usp=sharing

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