Project Title: Sketchfab Library of Augmented-Reality Compatible 3D Resources for Undergraduate Organic Chemistry Education

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Note to reviewers: My proposal does not describe a traditional scientific research project but rather a creative endeavor to develop scientifically rigorous educational resources that are superior to existing tools. In addition, as described in the **Next Steps** section, this work has exciting potential for a follow-up research project that measures educational outcomes in the classroom.

Background, Objective, and Significance

Organic chemistry (OChem) is a visual science. Learning OChem can pose unique challenges to students as it demands a solid understanding of the 3D structure of molecules.[1] The structure of a molecule is important because it determines the molecule's characteristics and reactive behavior.[2] It shouldn't be surprising that students with high visuospatial ability – the ability to mentally process and manipulate spatial forms – tend to do better on OChem problems.[1,3] Furthermore, educational tools that aim to improve and leverage students' visuospatial abilities lead to improved academic performance.[1,4,5] OChem is also a dynamic science that involves changes in chemical systems. For this reason, dynamic visuals, such as animated videos, may pose a pedagogical advantage over static images.[6,7]

Due to their ease of production and dissemination, two-dimensional symbols representing molecules are most often used to teach OChem.[8] Although they are convenient to print on paper and draw on a chalkboard, these abstractions are incomplete and can differ significantly in the information they contain.[9] In textbooks, these are often supplemented by computer-generated images that offer additional information but are static nonetheless. As a result, many students hold incomplete and static mental models of dynamic chemical processes.

To address this learning gap, various 3D educational resources are commonly used. These include physical model kits, which offer students hands-on, tactile familiarity with molecules,[10] molecular simulation software such as MolView,[11] Spartan, and Mol4D,[12] and animated videos uploaded to online platforms such as YouTube.[13] Unlike 2D images, these resources showcase molecules from multiple angles, deepening students' visuospatial understanding.[12] Model kits have well-established educational benefits[10,14] but can pose a financial burden to the student and are cumbersome to use. Simulation applications are highly interactive but often have high costs and steep learning curves.[12] Video animations are usually free and easily accessible but are not interactive. Additionally, animations uploaded to video-sharing sites such as YouTube are seldom vetted for quality and accuracy.

Some chemistry animation libraries, most notably ChemTube3D,[15] combine positive aspects of model kits, simulation software, and video animations. On ChemTube3D, users can freely rotate and zoom the models as the animation plays, making the animations more interactive than standard videos. The animations are made using computational chemistry methods[12] and are thus scientifically accurate. However, the resolution quality of the animations is relatively poor, and the website's layout can be confusing. Multistep reactions are divided into independent animations that must be played separately, making it difficult to grasp the whole, cohesive process.

There is a clear unmet need for additional 3D educational resources geared toward OChem students that are high quality, interactive, and scientifically accurate. Moreover, resources should be easily integrated into existing curricula to encourage adoption by instructors. In 2021, Aristov et al. created a library of 3D visuals illustrating introductory chemistry topics on the 3D model-sharing website Sketchfab.[16,17] The Sketchfab platform is highly interactive, allowing viewers to pan, zoom, and rotate models and fast forward, rewind, and pause animations. Sketchfab also supports high-resolution models and includes various 3D customization settings, such as lighting and material editing, to increase visual quality and appeal.

3D resources uploaded to Sketchfab are highly accessible, with several possibilities for integration into existing college courses. Students may easily view models on a computer display or using augmented reality (AR) on their smartphone or tablet. In recent decades, AR – the overlay of digital objects onto the user's natural surroundings – has emerged as a powerful educational modality that increases student motivation and understanding.[18] Sketchfab models can also be easily embedded into class webpages, online textbook resources,[19] and PowerPoint presentations. Although PowerPoint does not support custom animations, 3D files can be inserted and animated using a simple 'turntable' animation, which provides a smooth 360-degree view of the model.

I propose the creation of a free, AR-compatible Sketchfab library of scientifically rigorous, high-resolution 3D models and animations that illustrate key undergraduate-level OChem concepts. This creative pursuit will benefit OChem instructors and students who seek highly accurate and accessible educational resources. It will also provide a

streamlined workflow for creators who want to produce and publish cutting-edge 3D chemistry materials. I am excited to pursue this project to deepen my understanding of OChem and the exciting fields of computational chemistry, scientific visualization, and 3D computer graphics.

Methodology

I will expand the library sequentially, developing one specific model or animation at a time. Regarding OChem subject material, the library will roughly correspond to the AS.030.205 and AS.030.206 courses at Hopkins (OChem I and II). The software applications that will be used are Avogadro (molecule builder), ORCA (quantum mechanical software), ChimeraX (molecule visualization), and Blender (3D computer graphics tool). The following methods are partially adapted from Aristov et al.[16] I will perform all of these steps individually, not as part of a group/lab.

The first step will be identifying a suitable OChem topic or reaction for 3D visualization. To this end, I will defer to my mentor to provide his perspective as an OChem instructor. I will also review the course syllabus and lecture slides.

Next, I will use the software Avogadro to build approximate geometries for the molecules involved in the selected process or reaction. Avogadro is user-friendly and allows users to click and drag on the interface to quickly construct the molecule of choice. After creating the molecule, I will use the 'Optimize Geometry' function to adjust the atoms to a more energetically favorable arrangement. This is done to approximate the state of the molecule as it would most likely be found in nature. I will export the resulting geometry as a .inp (input) instructional file for use by ORCA.

I will use ORCA to further optimize the molecular geometry and calculate information about the molecule's energy, molecular and natural bond orbitals (informally described as 'electron clouds'), and charge distribution. When the selected process is a reaction, I will perform a 'relaxed surface scan' or a 'nudged elastic band' using ORCA commands to calculate the trajectory of the reaction. The choice of procedure will depend on the specific process being modeled. The results of these calculations will be automatically stored in several file types, namely .xyz files (contain the identities and optimized Cartesian coordinate positions of the atoms), .gbw files (describe the quantum state of the system), .cube files (describe charge distribution), and .out files (used for visualization). To maintain consistency, I will use the revPBE functional and def2-SVP basis set (quantum mechanical functions that describe electron density) for all calculations.

To visualize the molecules, orbitals, and electrostatic potential maps (colored surfaces that describe charge distribution), I will open the .out file in ChimeraX along with any .cube files. I will convert the molecule to a 'ball-and-stick' model in ChimeraX and the atoms will be colored by element. I will generate orbitals using the ChimeraX 'Orbital Viewer' and set them to the 95% isosurface (the boundary inside which an electron may be found with 95% probability). To generate electrostatic potential maps, I will use the 'Calculate SCF Electron Density' function to generate the 95% isosurface, color the surface using the .cube map, and set the surface to 50% transparency so the molecule remains visible. I will export molecules and orbitals as .x3d (Extensible 3D) files and electrostatic potential maps as .glb (GL Transmission Format) files.

To perform model cleanup, I will open these .x3d and .glb files in Blender. I will 'retopologize' the models, or make them more geometrically uniform, to eliminate deformations and visual artifacts. If needed, I will manually add double and triple bonds as they are not included in the .x3d and .glb files. I will export the finished model as a .fbx (FilmBox) file, which will be directly uploaded to Sketchfab. I may choose to prepare animations using Blender animation tools or by stitching individual .fbx 'frame' files together using Sketchfab's 'Timeframe' functionality. .fbx files are Microsoft Office compatible and may be inserted seamlessly into any Word or PowerPoint file. Using the Sketchfab 3D editor, I will make final adjustments to the model, such as lighting and material changes, as well as adjustments to the model's orientation, position, and scale. I will add a title and text description to each model and publish them under a Creative Commons Attribution copyright license.

Potential Roadblocks: I have demonstrated the project's feasibility by producing some sample models and animations, which can be found under my Sketchfab username "brianlei" (https://sketchfab.com/brianlei).[20] Screenshot stills of two of these works are showcased at the end of the proposal (**Figure 1** and **Figure 2**). The major difficulty that I experienced was in producing lengthy animations. The two currently uploaded animations were very time and labor-intensive because I used Sketchfab's 'Timeframe' functionality, which requires each frame to be individually prepared and stitched together. I hope to expedite this process for future animations by creating the animation using Blender, eliminating the need to design individual frames. Additionally, this would lead to much smoother animations since Blender can 'interpolate,' or fill in the gaps between each frame calculated by ORCA. Other potential challenges include brainstorming suitable topics for visualization, combining different information in a single animation (such as molecular

orbitals and electrostatic potential maps simultaneously), and dealing with long computation times. Certain ORCA calculations, particularly relaxed surface scans and nudged elastic band, can take several hours to complete and could potentially bottleneck production efforts. I hope to use the award to acquire better hardware, which would significantly reduce this downtime, as well as to purchase necessary software packages such as NBO 7.0 (ORCA plugin used to calculate natural bond orbitals.)[21]

Timetable: Before or in the early stages of the summer, I will review the AS.030.205 and AS.030.206 course curricula and work with my mentor to create a comprehensive list of ideas to be developed. For the remainder of the summer, I will dedicate the necessary amount of time each week to stay on track for completion by the end of the summer. It is difficult to estimate how long a given model or animation will take for me to complete, but animations will require substantially more time than static models. I will arrange weekly meetings with my mentor over Zoom to discuss progress and receive feedback. I plan to expand this library in the future, depending on my continued interest and availability.

Anticipated Results: This project will culminate in a comprehensive library of interactive 3D resources for OChem education, uploaded to the Sketchfab website under the username "brianlei."[20] This library will consist of compelling 3D models, static and animated, of atomic and molecular structures, orbitals, electrostatic potential maps, animated diagrams and graphs, and other useful visualizations. Each resource will be accompanied by a descriptive text caption. These resources will be free for reproduction (e.g. on websites, Word and PowerPoint documents, and augmented reality) and use by anyone, anywhere.

Next Steps: The most promising avenue of future work is integrating these resources into existing OChem courses, particularly AS.030.205 and AS.030.206. At this early stage, my mentor has expressed considerable interest in new instructional tools. In turn, I have suggested some ways to facilitate this integration, such as pasting 3D models into PowerPoint presentations or compiling them in a simple website that would be shared with students via the learning management system Canvas. Thus, there is excellent potential for a follow-up research project to measure the practical effectiveness of these resources in a classroom environment. For example, I could examine the relationship between time spent interacting with the 3D library and test scores. Also, surveys may be distributed to students as part of the end-of-semester course evaluation to qualitatively measure student attitudes toward the new 3D resources.

I may continue developing resources for the library indefinitely if any topics still need to be addressed. I may also expand the scope of the library to cover other disciplines, such as inorganic chemistry or biochemistry. I have no current plans to submit or publish outside of DREAMS, but I would be interested in doing so to increase the library's visibility. Overall, this creative experience will provide a strong foundation for future work in scientific visualization and communication, as well as research involving computational chemistry (synthesis, drug development, proposal of novel reaction mechanisms, etc.).

Supplementary Figures

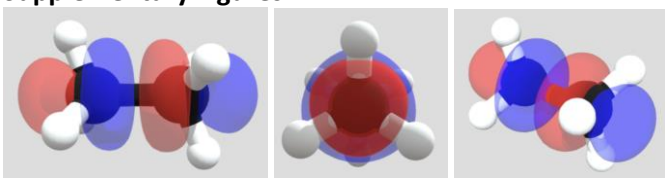

Figure 1. Three different viewing angles of the static model titled "sigma antibond". The antibonding molecular orbital of the molecule ethane is depicted in semi-opaque blue and red.

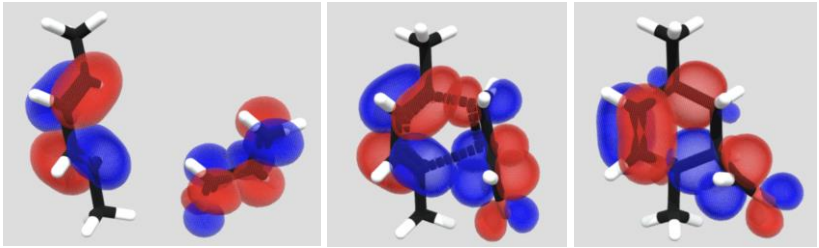

Figure 2. Three frames from the animated model titled "Diels Alder Reaction," showcasing the trajectory of a commonly taught OChem reaction. The molecule's natural bond orbitals are depicted in semi-opaque blue and red.

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