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Technology Report

Library of 3D Visual Teaching Tools for the Chemistry Classroom Accessible via Sketchfab and Viewable in Augmented Reality

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ABSTRACT: Through the implementation of the free website/smartphone application Sketchfab, we have found a simple means to introduce 3D visual tools into the chemistry classroom. Sketchfab stores 3D models and animations with free cross-platform accessibility. Blender is a free 3D modeling tool that has been used to prepare models and animations for dissemination via Sketchfab. By combining these two tools, we have created and are currently maintaining an ever-growing free library of interactive 3D models on various chemistry topics. Through the Sketchfab smartphone application, these models are viewable in augmented reality on most devices. Topics include molecular motion, isomerism, molecular orbital theory, chirality, and polymerization.

KEYWORDS: *High School/Introductory Chemistry, First-Year Undergraduate/General, Internet/Web-Based Learning, Multimedia-Based Learning, MO Theory, Polymerization*

INTRODUCTION

Teaching in a purely virtual setting as a consequence of the COVID-19 pandemic has encouraged the invention and adoption of new visualization tools.[1,2] Previous efforts have built libraries of freely accessible online teaching resources for chemistry.[3−5] These tools are particularly vital for a hands-on science like chemistry, in which the act of physically manipulating molecular models can be crucial for understanding spatial relationships.[6−8] For this purpose, molecular model kits, computational chemistry programs, and augmented reality tools have been increasingly introduced into the general chemistry classroom as teaching tools.[9−18] Model kits enable students to craft molecules physically, thereby discovering things like the effect of steric encumbrance, rotation about single bonds versus double bonds, and the nonsuperposition of enantiomers. Augmented reality offers a middle ground between the intangible computer-generated images and the tactile nature of model kits.[19−21] By coupling this tactile learning with visualization of the complex geometries inherent to molecular orbitals, students achieve a more holistic view of bonding in chemistry.[22−26] Unfortunately, computational chemistry tools often have a steep learning curve, may lack compatibility across operating systems and devices, and may require technical capabilities that many students lack.[27] To circumvent these problems, we have sought a universally accessible tool for manipulating 3D objects that can be implemented both in a virtual learning environment and in the physical classroom of high schools and universities, where a majority of students (>80% for high school and >90% for university) have access to smartphones.[28,29]

To this end, we have created and are currently maintaining an ever-growing library of interactive 3D models that have been uploaded to the free 3D model sharing website, Sketchfab.[30] This website offers a browser-based venue for viewing 3D models and animations, with interactive elements that allow the viewer to pan, zoom, rotate, and play/pause/rewind the contents of a 3D object or movie. Sketchfab allows for simple upload and distribution of these 3D models and animations across operating systems or devices, allowing mass distribution to a student body without concerns for compatibility. Furthermore, during the Sketchfab upload process, all models are automatically converted into a form that can be viewed through augmented reality via smartphone applications. This background feature of Sketchfab for augmented reality offers potentially one of the simplest means to create and integrate augmented reality models into teaching. We anticipate that these tools will remain relevant once in-person teaching returns to the norm, as students can download the Sketchfab smartphone application, available on

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Table 1. Selected Models Currently Freely Available on Sketchfab[a]

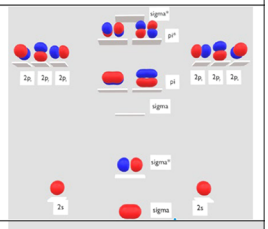
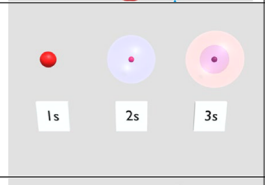
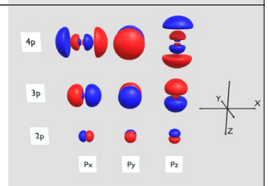
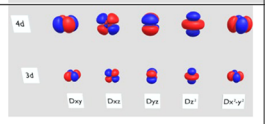
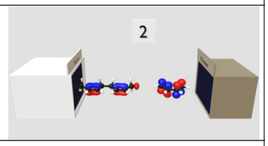
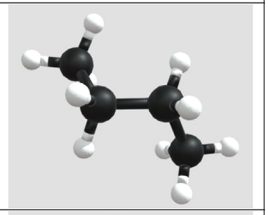
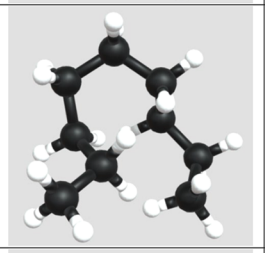
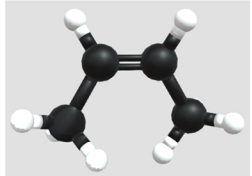
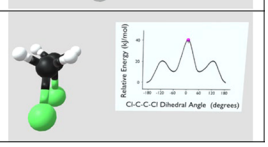
	Description	Snapshot
	MOs and AOs	
Molecular Orbital Diagram from Atomic Orbitals https://skfb.ly/6V9Lu	A diagram showing how 2*s* and 2*p* orbitals on F_2 combine to give rise to its MO diagram.	
1s, 2s, and 3s, Orbitals https://skfb.ly/6UAYF	A model showing the relative sizes and nodes associated with the first three *s*-orbitals.	
2p, 3p, 4p Atomic Orbitals on Xe: https://skfb.ly/6WQnr	A model showing the relative sizes and nodes associated with the first three sets of *p*-orbitals.	
3d and 4d Atomic Orbitals on Xe https://skfb.ly/6UDVU	A model showing the relative sizes and nodes associated with the first two sets of *d*-orbitals.	
1,3-Butadiene Polymerization https://skfb.ly/6UznK	An animation showing the orbitals of 1,3-Butadiene and the changes they undergo during an addition polymerization.	
	Molecular Motion	
Butane Rotation Smooth https://skfb.ly/6TwYN	A cartoon visualization of how butane can rotate about a C-C bond, and how this rotation affects the structure of butane.	
Rotation of Nonane https://skfb.ly/6TNq8	A cartoon visualization of how distorted nonane can appear when rotating about every C-C bond.	
Cis-2-Butene Rotation https://skfb.ly/6TJsN	An animation depicting the limited rotation in a hydrocarbon with a double bond.	
1,2-Dichloroethane Twist https://skfb.ly/6TOVy	An animation showing the energy levels associated with rotating about the C-C bond in dichloroethane.	

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Table 1. continued

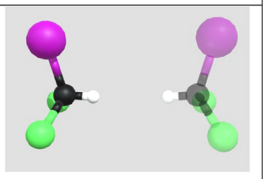
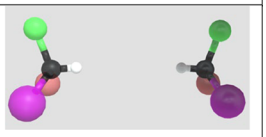
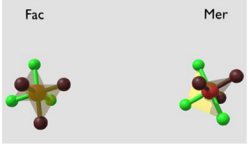
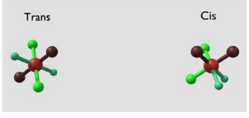
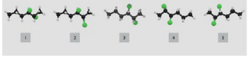
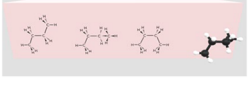
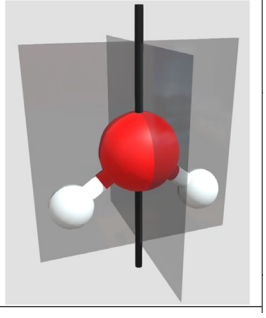
	Description	Snapshot
	Enantiomers and Chirality	
Superimposing Dichloroiodomethane Mirror Images https://skfb.ly/6XvoX	A simple animation showing dichloroiodomethane and its mirror image, followed by an overlap of the two molecules in 3D space. This animation demonstrates how non-chiral molecules can be superimposed.	
Enantiomers of Bromochloroiodomethane https://skfb.ly/6TJsW	A simple animation showing bromochloroiodomethane and its mirror image, followed by two attempts to overlap the molecules using only translation and rotation. The animation demonstrates how chiral molecules cannot be superimposed.	
	Isomers	
Fac/Mer Molecular Configurations https://skfb.ly/6ZDLv	A model showing the differences between the *fac* and *mer* isomers of a generic octahedral complex. Triangles were added for emphasis.	
Cis/Trans Molecular Configurations https://skfb.ly/onEQA	A model showing the differences between the *cis* and *trans* isomers of a generic octahedral complex.	
Structures of 2,3-Dichlorohexane https://skfb.ly/6UTsI	An animation showing five isomers of 2,3-dichlorohexane. The intent of this animation is for the student to try and identify which pair of isomers are identical, and which pairs are rotamers. This animation starts in a static pose, and the animation must be manually started through the user controls.	
Butane Rotation to Lewis Structure https://skfb.ly/6VTDB	An animation depicting four possible conformations of butane achieved by rotation about a C-C bond. Each conformer is shown sequentially with its associated wedge-dash structure.	
	Simple Symmetry	
Single Water Molecule https://skfb.ly/onwrI	A model of a single water molecule. Students are tasked with identifying all symmetry elements present in the molecule. By switching from a static model to display symmetry elements in bottom left of the user interface, the symmetry elements will be displayed.	

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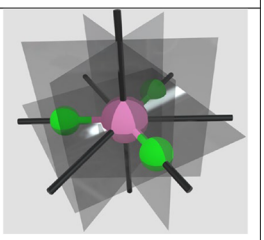
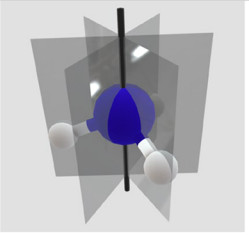
Table 1. continued

	Description	Snapshot
Single Boron Trifluoride Molecule https://skfb.ly/ootFs	A model of a single boron trifluoride molecule. Students are tasked with identifying all symmetry elements present in the molecule. By switching from a static model to action in bottom left of the user interface, the symmetry elements will be displayed.	
Single Ammonia Molecule https://skfb.ly/onw8w	A model of a single ammonia molecule. Students are tasked with identifying all symmetry elements present in the molecule. By switching from a static model to display symmetry elements in bottom left of the user interface, the symmetry elements will be displayed.	

[a]Each entry is accompanied by the model's title as found on Sketchfab, a URL, a short description, and a snapshot taken of the model or animation.

both Android and iOS. This smartphone integration allows students to view these models easily on screen in a classroom environment where a computer may not be convenient. Sketchfab also automatically generates embedded code, allowing for the models to be inserted directly into online open education resource (OER) textbooks and websites.[31] This embedding eliminates the need for students to navigate to alternative web pages or programs to view the 3D files.

Currently, our model library details common high school and general chemistry topics such as atomic orbital shapes, molecular motion, chirality and enantiomers, and molecular orbitals. We have limited the use of written descriptors to circumvent language barriers for international students. These models are currently freely accessible online through the Sketchfab website, and to date they have garnered over 6,400 views by chemistry teachers and students.

METHODS

All models were made and uploaded through a subset of four free software packages: ORCA,[32] Chimera,[33] Avogadro,[34] and Blender.[35] The models were later uploaded with a free account to Sketchfab, a browser-based 3D model hosting/sharing/viewing platform. Alternatively, 3D models that could be manipulated in Microsoft Office programs were directly exported from Blender, though these models lost their animations.

WORKFLOW

The quantum chemistry program ORCA was used to perform single point (SP) calculations on molecules and/or ions to derive their orbitals. Both natural bond orbitals (NBOs)[36] and molecular orbitals (MOs) were calculated from these SP calculations. To create output files that can be read by the molecular graphics program Chimera, surfaces of these orbitals were converted into .cube files using ORCA_PLOT with a standard file resolution of 100 grid points. This file conversion process also generated .xyz files that contained information about the molecule, specifically the atom types and positions, and this molecule was aligned with the orbital plots.

Visualization and manipulation of the orbital surfaces from the .cube files was performed in Chimera by loading both the .xyz and the .cube files.[33] The alias MySurface, generated by the line "MySurface volume all style surface level 0.05 color red level −0.05 color blue", was used to set the orbitals to the 95% isosurface and to set their colors. After initial visualization, the surfaces for each NBO and/or MO were saved as the wavefront object (.obj) file type, whereas the ball-and-stick structure of the molecule was saved as the collada (.dae) file type. Care was taken to not reorient the molecule when saving multiple orbitals through this method, as this reorientation would misalign the orbital's surface from the corresponding molecule's coordinates.

ALTERNATIVE WORKFLOW GUIDE

Another route for importing molecules in Blender is outlined in Dr. Joseph G. Manion's guide titled "Blender for Scientists—How to Make ANY Molecule in Blender".[37] This video provides an excellent step-by-step process for creating any molecule in Blender. Manion did not rely on any quantum chemical methods to make these models, and instead, he used the molecular mechanics algorithm embedded in the free Avogadro software package.[34]

BLENDER IMPLEMENTATION AND FINAL FILE EXPORT

After the 3D files were generated, they were imported into Blender where any remaining aesthetic changes and/or animations were made. These aesthetic changes include modification of an object's color, sheen, roughness, index-of-refraction, and opacity, as well as the refinement of lighting, scaling, and scene-composition. All animations were made through Blender's keyframe system by changing either the object's location, rotation, or scaling over a specified number of frames. These keyframed actions combined with object parenting were used to create animations like "Butane Rotation Smooth", which displays a perfect loop of every C−C bond rotating simultaneously and at different rates in a butane molecule.

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Microsoft Office365 compatible 3D files were made by exporting the Blender model as a filmbox (.fbx). These files can be directly inserted into any Word or PowerPoint file with their 3D nature preserved, allowing for real time rotation, scaling, and animation inside Office. It should be noted that some material attributes are lost, like the metallic value, when viewing 3D files in Office365, and we have found that simple base colors and α values (opacity) have worked best. A recent guide by Manion, titled "Blender for Scientists—Using 3D Objects Directly in PowerPoint", details an alternative process of generating 3D objects for use in PowerPoint, though this guide favors glTF 2.0 files and does not detail how α values can be used to incorporate transparent objects.[38]

Uploading models to Sketchfab was done either through a freely available Blender extension or by using the Sketchfab website directly. All models were uploaded to Sketchfab as Blender's default save file type (.blend). Once uploaded, Sketchfab's 3D viewer was used to make any final changes to individual materials in the model, which define the appearance of each object in the scene. These changes include scene lighting, initial camera location, model orientation, and scale and set the animation to autoplay upon loading. Once uploaded, these models were set to public, a title and description were added, and their copyrights were declared.

PEDAGOGICAL FRAMEWORK

Sketchfab automatically generates multiple styles of embed code for every public model on the website. These embed codes allow for simple integration into online resources frequently used in chemistry classes. These embedded files allow for finer control of the material viewed by students and help eliminate distractions and breaks in student workflow that may occur when students are asked to view multiple websites simultaneously.

CURRENT MODELS AND ANIMATIONS

All of the models we have made using the above procedure are available on Michael Aristov's Sketchfab account at https://sketchfab.com/Michael.Aristov. Table 1 offers a list of some of the models we have made. As we continue to generate more of these models, they will be added to the Sketchfab account. Additionally, all models are downloadable from the Sketchfab website as .blend or .glTF; all of the .blend files for the models described in Table 1 are included in the SI.

STUDENT IMPLEMENTATION AND CLASSROOM INTEGRATION

We believe these 3D teaching tools will offer significant benefits over their more classical 2D depictions. Specifically, we seek to replace the static 2D figures of complex systems commonly found in textbooks with dynamic and interactive 3D models. We have started pursuing this replacement by including these 3D models into the open education resource (OER) chemistry textbook preclass materials for Advanced General Chemistry, Chem 109, at the University of Wisconsin—Madison.[31] Several example pages with these embedded 3D models from the above OER textbook that was used to teach the Fall 2020 chemistry course at UW Madison are provided here.

- Molecular Conformations: https://wisc.pb.unizin.org/chem109fall2021ver02/chapter/conformations/
- Cis−trans Isomers: https://wisc.pb.unizin.org/chem109fall2021ver02/chapter/stereoisomers-geometric-isomers/
- Enantiomers: https://wisc.pb.unizin.org/chem109fall2021ver02/chapter/stereoisomers-enantiomers/

Because these animations were embedded into an OER, we cannot attribute learning gains to the animations separately. However, there is a positive correlation between exam scores and time spent using the OER.

We propose that these 3D models should be used instead of classical 2D figures in online textbooks. For classrooms with physical books, we suggest emailing links to the models as appropriate throughout the course or embedding them in a course webpage. For interactive work, we suggest allowing students to work in small groups and to view the models on their smartphones with the task of answering scaffolding questions about the model. An example of this type of task is seen in the single water molecule model (https://skfb.ly/6UTsI), where students would be asked to identify all symmetry elements for the water molecule. The students can view the correct answer by selecting "display symmetry elements" in the Sketchfab user interface.

CONCLUSION

This technical report highlights a new and growing library of 3D models and animations that can be viewed on any device, which thereby allows for simple integration across a variety of learning environments. The animation capabilities of Blender simplify the creation of novel visualizations for otherwise esoteric descriptions of chemistry concepts, like a chiral molecule's inability to be superimposed on its mirror image or how multiple wedge−dash structures can be drawn for different conformations as seen in Table 1. The free nature and ease of use inherent to Sketchfab allow for students to view these models via computer display or augmented reality. This combination of Blender and Sketchfab provides a simple means by which an instructor can create and distribute 3D teaching tools for any class. Our initial work has focused on the integration of these models as additional teaching tools in the classroom, and these models have gathered over 5,800 views from students and teachers alike in the 14 months that they have been publicly available.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.1c00460.

Finalized project files for all models and animations shown in Table 1 as output from and modifiable in Blender (ZIP)

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Notes

The authors declare no competing financial interest.

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