3D Printing of Molecular Models

Gregory Thompson and Dr. Kevin McWilliams

Department of Chemistry and Biochemistry, Gupta College of Science, Coastal Carolina University

Abstract

Molecular structures, spatial arrangements, bond angles and stereochemistry are examples of topics that chemistry students struggle to grasp because it can be difficult to visualize how they work. 3D printing offers a way for instructors to provide students with molecular models to allow them to experience hands-on learning to better understand these concepts. The aim of this research is to design a method of remotely monitoring as well as controlling the 3D printer, and to explore what molecular editing programs could be useful in creating 3D models to print. To address the former, the software, Octoprint, will be used in conjunction with a Raspberry Pi controller and camera. To address the latter, the molecular editor, Avogadro, will be used, in conjunction with other software to produce STL. files which can be utilized by the printer. Our goal for this semester is to have the 3D printer fully operational and to be able to design our own molecules and print them out so that students can have access to handheld versions of complex molecules when learning spatially challenging concepts.

Objectives

- Develop a method of remotely monitoring and controlling the 3D printer by using Octoprint and a Raspberry Pi device paired with a camera.
- Explore software that allows for the design of molecules, such as Avogadro.
- Develop a method that can convert the molecule produced into an .stl file, so that it can be printed with the 3D printer.

Methods

- Avogadro is used to create the molecular model and optimize bond angles.[1]
- Avogadro 2 is used to produce a VRML file.[1]
- Multiple failed attempts to produce a VRML and STL. file with several different programs including Python Molecular Viewer.[2]
- Meshlab is used to convert the VRML into an STL. file.[3]
- The STL. file can then be imported to Cura and printed.
- Raspberry Pi device and OctoPrint and a Camera.[5,6.]
- An alternative method involves a Teckin smart plug and a Wyze Camera.
- Raspberry Pi is a better method, but the alternative is much cheaper.

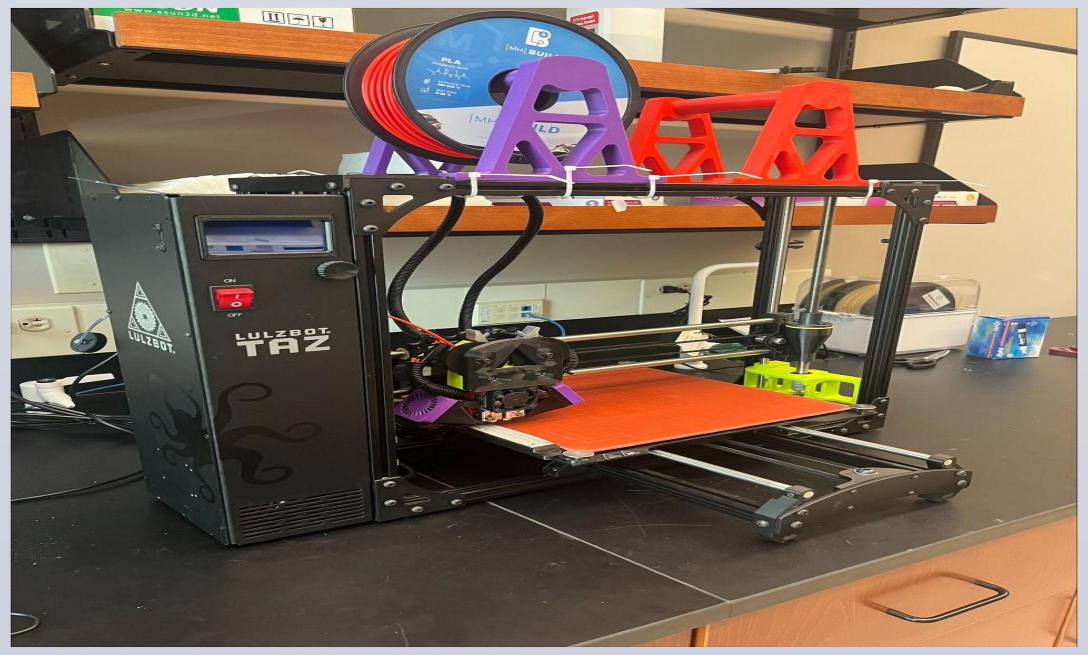

Figure 1: Photo of the Lulzbot Taz 6 3D printer.

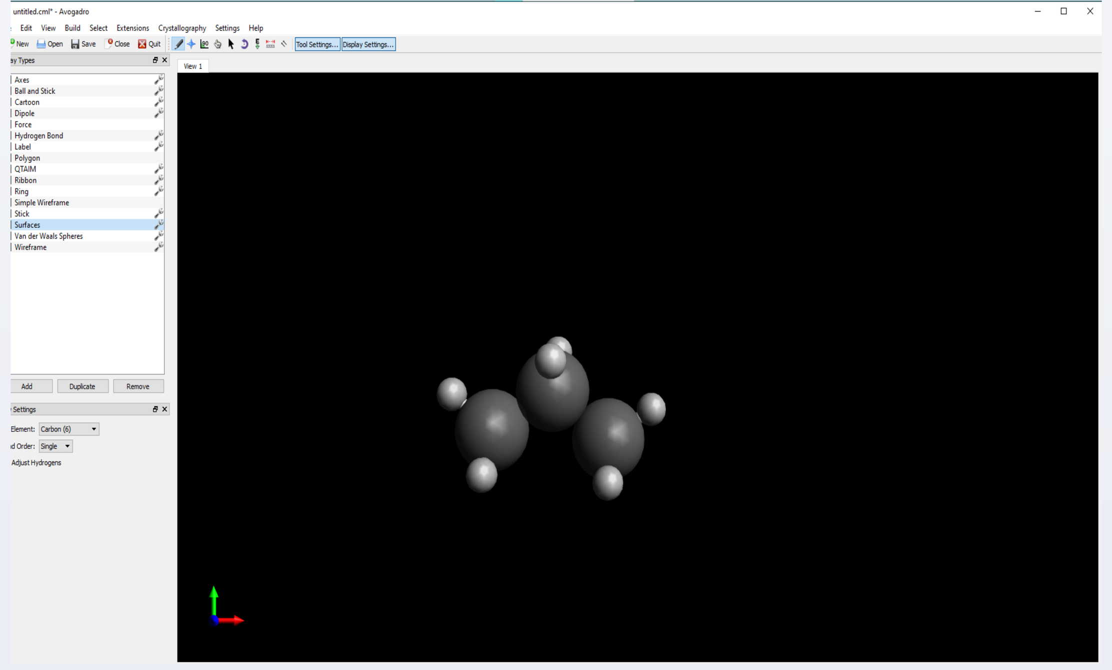

Fig. 2: Model of propane (C3H8) built within the program, Avogadro.

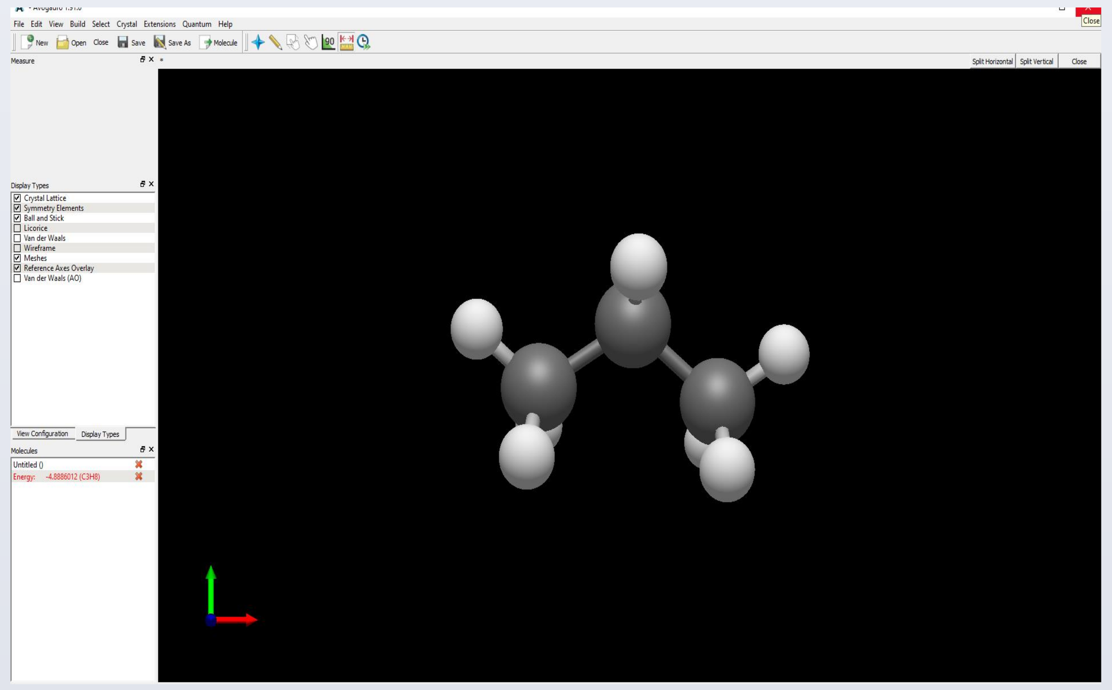

Fig. 3: Model of propane (C3H8) optimized within the program, Avogadro 2.

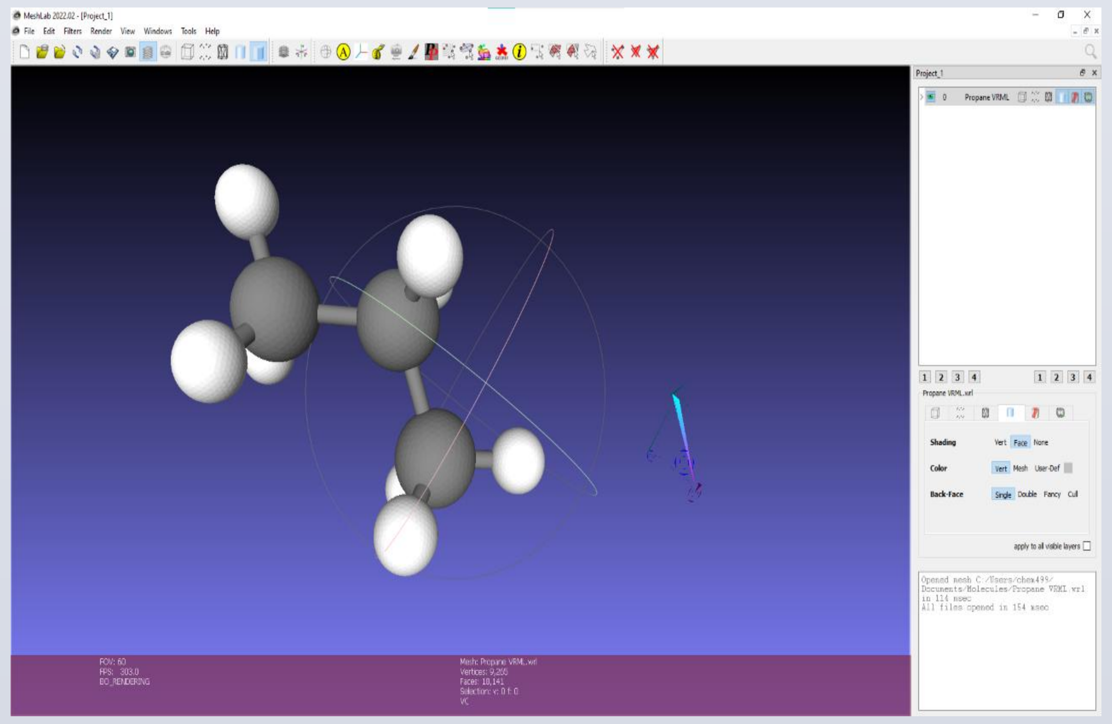

Fig. 4: Model of propane in MeshLab.

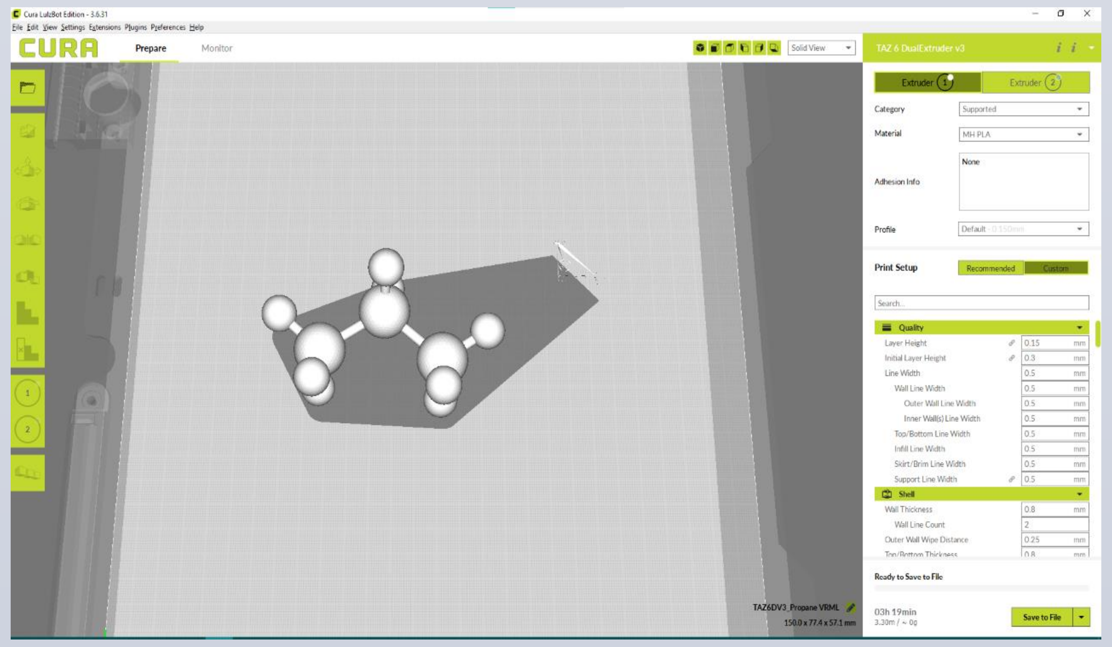

Fig. 5: Model of propane ready for print in Cura.

Fig. 6: Raspberry Pi device that is necessary to use Octoprint.

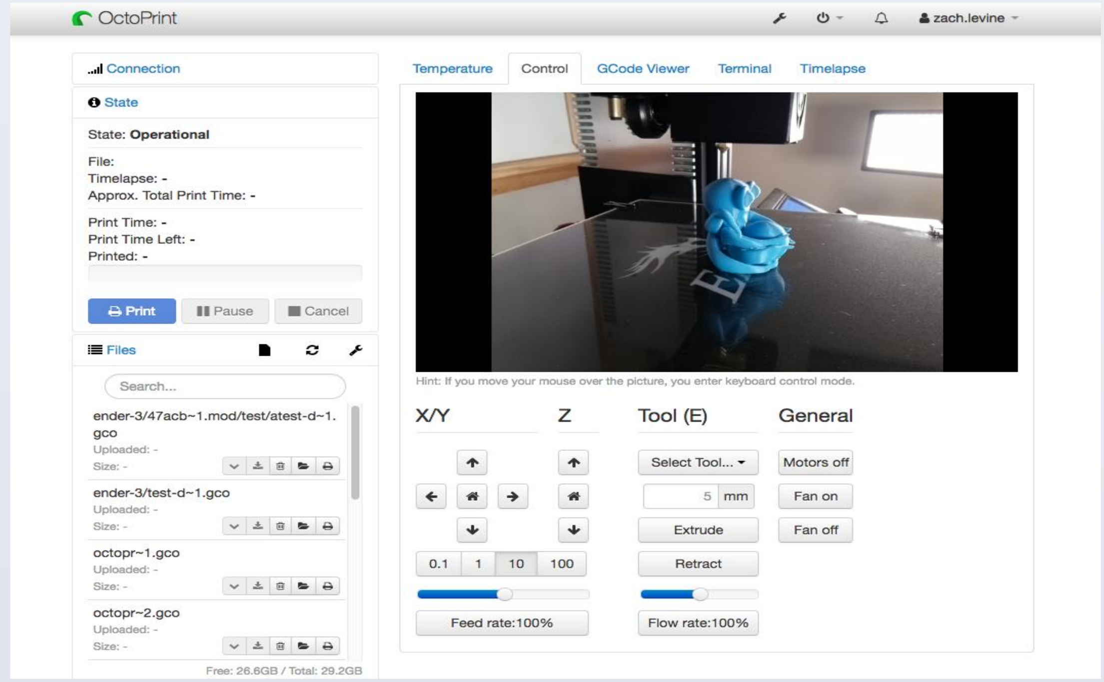

Fig. 7: User view of the Octoprint program, monitoring a print.

Fig. 8: Wyze Camera that could be used to monitor a print.

Fig. 9: Teckin smart plug that could turn off the printer.

Discussion

- Avogadro and Avogadro 2 were successfully able to be used together to produce an accurate molecular model with proper bond angles and lengths.
- Avogadro can be useful in producing multiple different kinds of complex molecules, including DNA, RNA, and amino acid chains, suggesting that our research will be helpful for Biology instructors as well.
- MeshLab was successful in converting the molecular model into an STL. file. Python Molecular Viewer was not successful for us. Chimera was also not successful.
- The STL. file produced by MeshLab was able to be imported successfully into Cura.
- However, no models were able to be printed this semester due to issues with the printer itself.
- Although two different methods were designed for remotely monitoring and controlling the printer, neither were able to be implemented at this time.
- However, a good foundation was set for the next students who take over this project. It is likely the printer will be fully operational including remote monitoring next semester.

References

1. Marcus D Hanwell, Donald E Curtis, David C Lonie, Tim Vandermeersch, Eva Zurek and Geoffrey R Hutchison; “Avogadro: An advanced semantic chemical editor, visualization, and analysis platform” Journal of Cheminformatics 2012, 4:17.
2. Michel F. Sanner. Python: A Programming Language for Software Integration and Development. J. Mol. Graphics Mod., 1999, Vol 17, February. pp57-61
3. Cignoni, P., Corsini, M. & Ranzuglia, G. (2008). MeshLab: an Open-Source 3D Mesh Processing System.. ERCIM News, 2008.
4. Segarra, V. A., and Chi, R. J. (2020). Combining 3D-Printed Models and Open-Source Molecular Modeling of p53 To Engage Students with Concepts in Cell Biology. J Microbiol Biol Educ 21.
5. Richardson, M., & Wallace, S. P. (2012). Getting started with Raspberry Pi. Sebastopol, CA, O'Reilly Media.
6. Häußge, Gina (24 May 2022). "New release: 1.8.1". OctoPrint.org. Retrieved 26 June 2022.

Acknowledgements

We would like to thank Coastal Carolina University and the Department of Chemistry and Biochemistry for providing the funds and support to perform the research done this semester.