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App-Free Method for Visualization of Polymers in 3D and Augmented Reality

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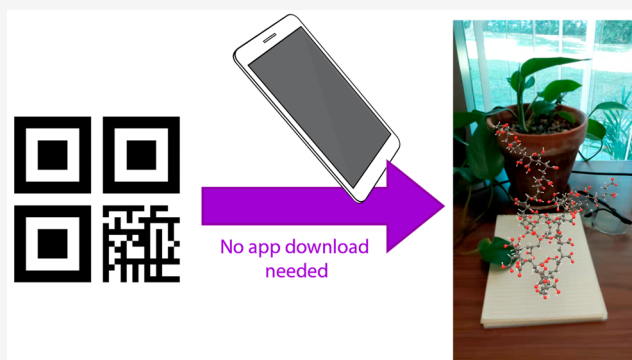
Article Recommendations



Supporting Information

ABSTRACT: The rise of virtual and online education in recent years has led to the development and popularization of many online tools, notably three-dimensional (3D) models and augmented reality (AR), for visualizing various structures in chemical sciences. The majority of the developed tools focus on either small molecules or biological systems, as information regarding their structure can be easily accessed from online databases or obtained through relatively quick calculations. As such, due to a lack of crystallographic and theoretical data available for nonbiological macromolecules, there is a noticeable lack of accessible online tools for the visualization of polymers in 3D. Herein, using a few sample polymers, we showcase a workflow for the generation of 3D models using molecular dynamics and Blender. The 3D structures can then be hosted on p3d.in, where AR models can be generated automatically. Furthermore, the hosted 3D models can then be shared via quick response (QR) codes and used in various settings without the need to download any applications.

KEYWORDS: *Computer-based Learning, General Public, Upper-division Undergraduate, Web-based Learning, Solids, Polymer Chemistry*



INTRODUCTION

The three-dimensional (3D) structure of molecules is a key factor in understanding the physical and chemical properties of materials (e.g., reactivity, melting point, optical properties, etc.). As such, physical models are often used by lecturers and students to help with the visualization of a chemical species. Augmented reality (AR) and 3D models are accessible tools that are slowly gaining traction within the chemical and biochemical communities.^{1–3} For example, these tools have been used to enhance learning and safety practices in the laboratory^{4–8} and to provide an engaging and interactive way to visualize chemical species.^{9–16} For these visualization technologies, a limited number of models and animations are created and accessed via a mobile application, Web site, or quick response (QR) codes.^{6,7,9,10,13,15–19} Typically, these models consist of small molecules (~100 atoms or less) represented as atomistic models or large molecules such as proteins represented as simplified models like “ribbons” and “sheets”. The data used for creating 3D models of these systems can be easily accessed via databases such as the Cambridge Crystallographic Data Base²⁰ or the Protein Data Bank.²¹ Alternatively, geometric information could be obtained through relatively straightforward computational methods. On the other hand, polymers, with molecular weights in between small molecules and biological macromolecules, remain largely unrepresented, likely a result of the limited information available for their visualization. Although there are

well established libraries of 3D polymer structures on the web (namely 3dchem.com and pslc.ws), they offer either a small but detailed set of polymers or a vast set of oligomers with no AR visualization option. Additionally, these tools may not offer the specific polymer that one may look for (i.e., specific degree of polymerization or tacticity). In this work, through a series of sample polymers, we showcase a workflow for creating an app-free visualization method of any polymer to lower the integration barrier of using this technique in educational settings (Figure 1). We hope that our models demonstrate the utility of this workflow and establish it as a practical and flexible visualization approach for similarly sized systems. Furthermore, by hosting our models on platforms such as p3d.in and sharing them using QR codes, we can make the interactive models accessible to anyone with a smart device and Internet access.

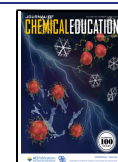
Obtaining Chemical Information

We included a detailed guide used for obtaining and processing the chemical data as [Supporting Information](#). Molecular

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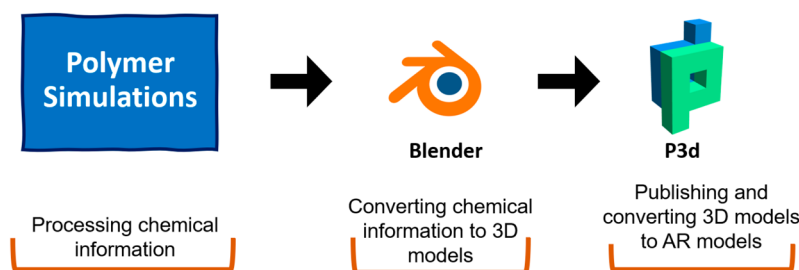


Figure 1. A graphical summary of our workflow: Simulations are performed to obtain chemical information and then converted into 3D models to be hosted on p3d.in for visualization and AR processing.

dynamics (MD) simulations were carried out on the polymers shown in [Table 1](#) with input files and initial configurations that were generated expediently with a coarse-grained (CG) resolution using CHARMM-GUI's *Polymer Builder*.^{22–25} In this workflow, a CG model of polymeric chains containing 50-mers (except in the case of polystyrene, 25-mer) is solvated in a water box, equilibrated for 20 ns at 300 K using OpenMM²⁶ (the default λ value is used for nonbound interaction strength), and then replaced with all-atom relaxed topologies. Next, the atomic structures are minimized and equilibrated, first in the canonical ensemble (NVT), then in the constant-pressure ensemble (NPT) with time steps of 1 and 2 fs, respectively, using the open source large-scale atomic/molecular massively parallel simulator (LAMMPS) code.²⁷ Finally, the AR models corresponding to each polymer are generated as described below using snapshots that can be taken from the NPT simulation step. Unlike small molecules, polymers do not have a single “most stable” conformation, they have many possible conformations with close energies. Therefore, only a snapshot is used based on the user's liking. A snapshot in this case refers to a polymer conformation at a specific time.

The computational cost and effort of this procedure can be dramatically simplified if one is simply interested in generating polymer structures for pedagogical purposes (as opposed to probing specific intermolecular interactions), in which case, doing atomistic simulations may not be necessary and a more coarse picture could suffice.²⁸ In this situation, the user can directly download the desired all-atom replacement of the CG model structures that are generated interactively by CHARMM-GUI or perform a quick force field optimization using tools such as Avogadro²⁹ and render them without the need for running dynamical simulations on a local computer or a computational cluster.

Converting Chemical Information into 3D Models

A step-by-step guide for using Blender is included in the [Supporting Information](#). The saved .pdb file is imported into Blender using the Atomic Blender plugin by Clemens Barth.³⁰ If bond information is missing from the .pdb file, converting it into an .xyz file and then back into a .pdb file in Avogadro fixes the problem. By merging and deleting unnecessary objects (i.e., caps at the ends of bonds), the number of vertices used for the representation of the 3D model is lowered such that a smaller file size is obtained. A smaller number of vertices and file sizes are crucial for allowing the 3D models to be hosted online and processed into AR models. The number of vertices of the 3D model can be further reduced if the polymer model is large by merging nearby vertices by a larger distance or by using the “Decimate” modifier tool in Blender. Either method reduces the quality of the models, so it is important to use them sparingly.

We recommend following the YouTube tutorial by CG Figures, “*Blender for Scientists – How to Make ANY Molecule in Blender*” for a general step-by-step guide.³¹ An example of the files generated for [Table 1](#), entry 9 can be found in the [Supporting Information](#).

Publishing and Converting 3D Models to Augmented Reality

Once the 3D model is colored and finalized, the model is exported as an .fbx file; .fbx files can be downloaded and opened on a computer. These files will allow the user to interact with the 3D structure by using the mouse even though the AR experience cannot be obtained. In order to get the AR experience, the .fbx file should be uploaded to the hosting platform of choice. We used p3d.in for visualization purposes and automatic conversion to AR models. Once the file is uploaded, the URL to each model is converted into a QR code using a QR code generator (we used www.qr-code-generator.com), which allows an easy sharing of the AR models.









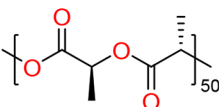





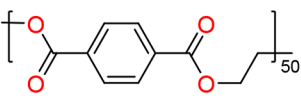



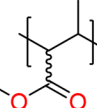



CURRENT MODELS

A complete list of the 3D models created at the time of writing of this work is presented in [Table 1](#). Upon scanning any of the QR codes using a smart device's default camera app, the user will be directed to the p3d page that is hosting the 3D model. The user can either interact with the model through their browser or, by enabling the AR function, use the built-in software on their smart devices to visualize and interact with the AR models ([Figure 2](#)). We do not recommend a third-party QR code reader application, but if the users are using a separate QR code reader app, they may need to manually go to the directed webpage on their phone browser after scanning the QR codes to get the full experience. In the future, additional models can be found on our Web site at www.cicchemistry.com/AugmentedReality.

APPLICATION AND RECEPTION

The generated QR codes were implemented in lecture material and presentations in an upper division polymer chemistry course consisting of 12 graduate students. This course introduces the concept of polymers, their syntheses, characterization, properties, and advanced applications such as biomedical materials, 3D printing, and conductive polymers. At the beginning of the class, the concepts of polymers, polymer degradability, tacticity, and melt and glass temperatures were introduced and explored. The learning objectives of using the 3D polymer structures were to visualize polymer chains, understand how polymer chains coil, and understand the importance of substituents in determining tacticity. To gauge the reception of our tool in a classroom setting, we conducted an anonymous survey using Google Forms ([Tables 2 and 3](#)).

Table 1. Modeled Polymers

| Entry | Polymer | QR code |
|-------|---|---|
| 1 |  Polyethylene (high density) |  |
| 2 |  Poly(vinyl chloride) |  |
| 3 |  α -poly(styrene) ^a |  |
| 4 |  iso-poly(styrene) |  |
| 5 |  iso-poly(lactic acid) |  |
| 6 |  iso-poly(propylene) |  |
| 7 |  α -poly(propylene) |  |
| 8 |  Poly(ethylene terephthalate) |  |
| 9 |  α -Poly(acrylic acid) |  |
| 10 |  α -Poly(methylmethacrylate) |  |
| 11 |  Poly(ethylene oxide) |  |

^aDue to the large number of vertices associated with this structure, a 25-mer model was prepared instead of a 50-mer model.

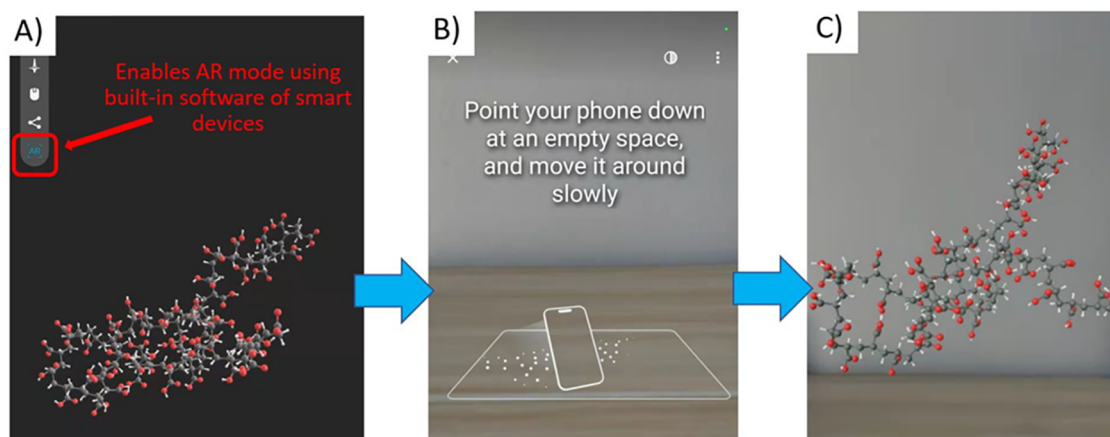


Figure 2. (a) Sample webpage after scanning a QR code. (b) Prompt given to the user after enabling AR mode via the smart device's built-in software. (c) AR model visualized on a desk.

Table 2. Gauging Prior Student Experience with 3D and AR Tools

| entry | prompt | true | false |
|-------|---|------|-------|
| 1 | Prior to this course, I have used 3D and/or augmented reality tools in a classroom setting. | 4 | 8 |
| 2 | Prior to this course, I was aware of other 3D and/or augmented reality tools related to polymers. | 2 | 10 |

Due to the small class size, we are unable to do any meaningful statistical analysis of the results. However, it is clear that the overall reception toward the utilization of this tool in a lecture setting is positive with 10–11 members of the class (Table 3, entries 5 and 6) suggesting that they benefited from this tool. We hope that other lecturers can implement their own custom-made macromolecular structures in lectures and outreach activities.

CONCLUSION

In this work, we showed that using a series of free and readily available resources, AR and 3D models for any short polymer chain can be generated. With the help of 3D file hosting platforms such as p3d and QR code generators, these macromolecules can be easily accessed as both 3D and AR models without the need of any downloaded applications, making this visualization method easily accessible to a wide audience that is in possession of a smart device and Internet access. The easily accessible and interactive nature of these models may be utilized in a variety of educational settings to create an engaging experience for students at all levels.

Table 3. Survey Responses from Students

| entry | prompt | strongly agree | agree | disagree | strongly disagree |
|-------|--|----------------|-------|----------|-------------------|
| 1 | Prior to using 3D and augmented reality tools, I was confident in visualizing polymer structures. | 2 | 3 | 6 | 2 |
| 2 | After using 3D and augmented reality tools, I am more confident in visualizing polymer structures. | 4 | 6 | 1 | 1 |
| 3 | Seeing 3D structures has deepened my understanding of polymers. | 3 | 7 | 2 | 0 |
| 4 | Being able to physically manipulate the structures on my electronic device has helped me make connections between what I know and what I'm learning. | 2 | 7 | 2 | 0 |
| 5 | I believe that seeing the 3D structures has helped me understand polymer properties such as tacticity better. | 3 | 7 | 2 | 0 |
| 6 | Overall, I believe 3D and augmented reality tools have enhanced my learning experience. | 5 | 6 | 1 | 0 |
| 7 | I would like to see more 3D and augmented reality tools used in future classes. | 4 | 6 | 1 | 1 |

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at <https://pubs.acs.org/doi/10.1021/acs.jchemed.2c01131>.

A detailed guide for using CHARMM-GUI and Blender, and files generated for Table 1, entry 9 (PDF)

Supporting fbxyz file (ZIP): Sample 3D model of Table 1, entry 9

Supporting pdb file (PDB): Sample snapshot from molecular dynamics simulations of Table 1, entry 9

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Notes

The authors declare no competing financial interest.

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