



# Modeling atoms and molecules using virtual reality

Juan Barron, Dr. Christopher Ivancic, Dr. Brian Barngrover

Stephen F. Austin State University, Department of Computer Science, Nacogdoches, TX 75962

Stephen F. Austin State University, Department of Chemistry and Biochemistry, Nacogdoches, TX 75962

## Abstract

It can be difficult to visualize the geometry of molecules in a 2-dimensional plane. We have built a tool that allows students to combine different elements to generate 3-dimensional models. This tool shows the proper geometry on their phones to assist in translating from an abstract valence model to a more accurate 3-dimensional one.

## Purpose

The purpose of the project was a way to show high school and freshman level chemistry students the different ways that atoms interact with each other to form molecules. There are other apps in the public that uses virtual reality to show molecules and atoms using trackers, but they are not showing the whole picture to students. The app uses the positions of the atoms to determine if the pattern meets the condition for the molecule to appear.

## Theory

The valence model of atomic structure is used as an introductory tool to help students visualize how the atoms combine to make molecules. As with most models, there is a loss of fidelity by showing it in a 2-dimensional plane. The actual 3-dimensional structure is different and can be hard for new chemistry students to visualize. This tool uses molecular geometry to produce an interactive 3-dimensional model of molecules.

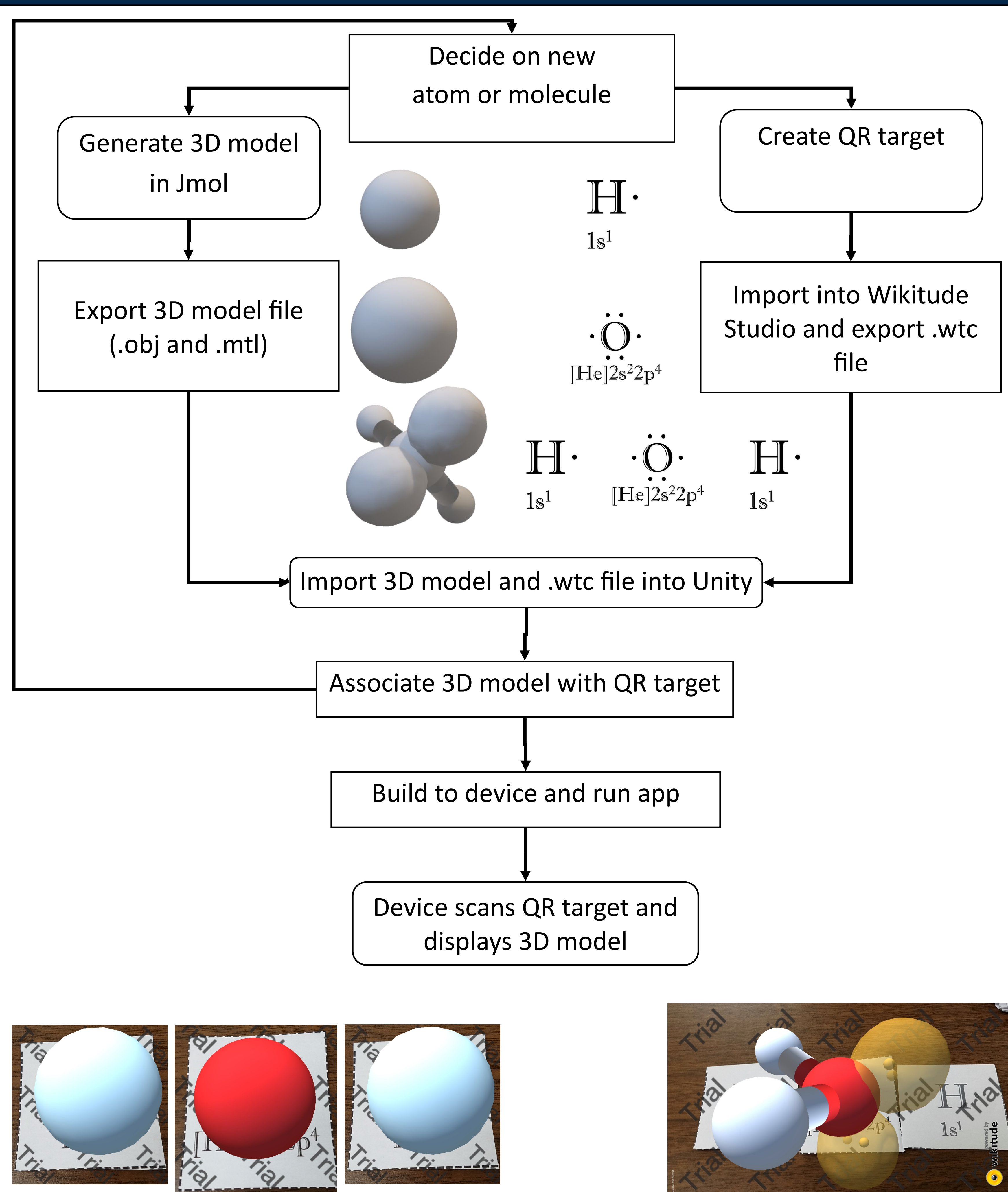
## Contacts

Juan Barron (barronjg1@jacks.sfasu.edu)

Dr. Christopher Ivancic (ivanciccp@sfasu.edu)

Dr. Brian Barngrover (barngrovbm@sfasu.edu)

## Results



## Methodology

The initial stages of the app produced a procedure to read predefined QR codes and render a 3-dimensional atom. This atom appears on the app and allows you to rotate it through touch controls. The purpose of the app is to translate from traditional 2-dimensional structures to 3-dimensional ones.

The first challenge to overcome involved reading the QR codes in the proper order. For example: having 2 hydrogen and 1 oxygen QR codes to show a water molecule depends on the order the codes are placed. It is not good enough to just have the codes available. Since the app is supposed to show a translation between 2D and 3D models, the QR codes for water should be put together in the Valence form and the app needed to distinguish this particular placement over a random one. We accomplished the reading of the Valence placement by scanning a general geometry of the camera and had the app read the QR codes in a relative placement to one another.

Once we had a working example of water, the next big challenge was to develop a method of efficiently telling the app of different kinds of molecules and their structures. We accomplished this task by developing a structure to read configuration data once the app is launched. By creating this structure, any additions or changes to molecule data are made to the file without having to re-implement the application itself.

## Acknowledgments

- Stephen F. Austin Department of Chemistry and Biochemistry
- Stephen F. Austin Department of Computer Science
- Summer Undergraduate Research Experience
- Increasing Hispanic and Underrepresented Groups in STEM

## Conclusion

The project concluded with a working prototype with many different molecules it can read. The app works on most Android platforms and can distinguish between atoms of random placement or atoms with a Valence placement to produce a specific 3D molecule