

Visualizing the Properties of Carbon-based Molecules

Cameron D. Collins, Coastal Carolina University, Conway, SC 29526

Dr. Steven J. Stuart, Clemson University, Clemson, SC 29634

Dr. Joshua A. Levine, Clemson University, Clemson, SC 29634



Abstract

Most visualization tools used in chemistry are capable of visualizing basic properties such as bond distance, angle, etc, but lack the ability to visualize other more specific properties. The software developed as a result of this project measures chemical and mathematical properties that are exclusive to carbon-based molecules. *Processing* is a graphics-based programming language that uses *Java* syntax to build the software. The first step involved reading the file provided and developing a three-dimensional model. Next a *Processing* library was imported which allows the user to rotate and zoom in on the model. The final step was to develop a user interface which allows the user to select which properties he/she wants displayed, which will color the atoms, bonds, and rings based upon those properties. All of the properties being visualized are difficult to visualize without computer simulation making the use of color necessary. Future work will involve transferring the software to a language that is more reliable, such as *Python*, and making a more user-friendly graphical interface.

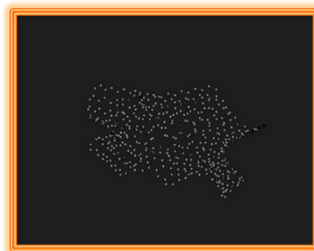
Motivation

There are not currently software tools to effectively measure the properties that the computational chemists are looking to measure. In order to do this, we are developing a program from scratch using the *Processing* language designed for visualization.

Methods

- Processing – a graphical extension of Java
- Used a data-file that consists of 3D coordinate points of a graphite molecule to develop a model
- Currently using vector math to calculate

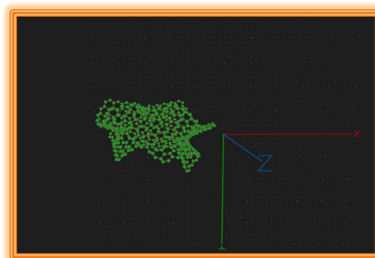
Results



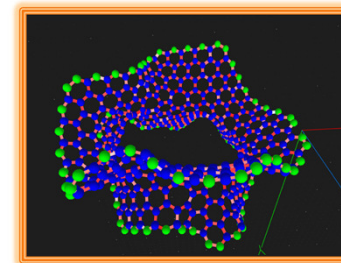
Read file, developed 2D model



Developed 3D model using coordinates in the file



Imported *proscene* library to add camera functionality and reference points



Measured and visualized bond length and coordination number

Future Work



Acknowledgements

REU Funded by NSF ACI Award 1359223
Vetria L. Byrd, PI



Advanced Visualization Division

