Middle/High School Science Case Study: Water Structure and Properties

NCSSM

Bob Gotwals
Computational Science Educator
gotwals@ncssm.edu
NCSTA Middle School and High School Webinar Series

January 27, 2021

NOTE! All of the materials for this case study are available on NCSSM's Gotwals Outreach page: `https://ncssm.instructure.com/courses/411`

North Carolina Standard Course of Study Objectives for Middle School Science The following objectives from the NCSCOS are potential targets for this case study.

- 6.P.2 Understand the structure, classifications and physical properties of matter.
- 8.P.1 Understand the properties of matter and changes that occur when matter interacts in an open and closed container.

- 8.P.2 Explain the environmental implications associated with the various methods of obtaining, managing and using energy resources.

1 Background

Water is the most essential molecule needed to sustain life, and is a good model for students to learn about the basic structure and properties of molecules. In this case study, students will apply the technologies, techniques and tools of computational science (scientific computing) to the study of the structure, properties, and behavior of the water molecule. Specifically, they will use computational chemistry methods, using a research-grade software package (Gaussian16) to conduct their studies.

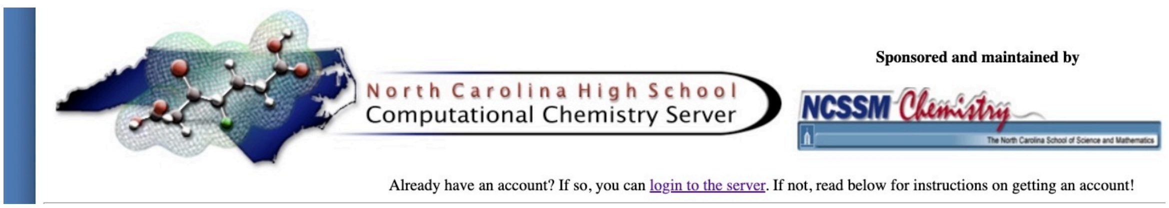

Figure 1: The North Carolina High School Computational Chemistry server

Figure 1 shows the top of the web page for the North Carolina High School Computational Chemistry server (`http://chemistry.ncssm.edu`), housed and maintained by the chemistry staff at the North Carolina School of Science and Math. The server provides free access to computational chemistry software, supported by an easy-to-use graphical interface known as WebMO. Using this server, students can build molecules (such as water), and conduct various structure and property calculations on that molecule. For example, in this case study, students will answer these questions:

1. What is the general structure of the water molecule?
    - General structure: water has a bent structure, and is a flat, or planar, molecule
    - Bond lengths: the bonds between the hydrogens and oxygen is slightly less than 1 angstrom ($\mathring{A}$), which is $1x10^{-10}$ meters)
    - Bond angle: the angle between the two hydrogens and oxygen is approximately 104.5° (degrees)

2. What are some of the properties of water?

    - Polarity: water has a dipole moment, a measure of polarity, with the pole running from oxygen (negative) to the midpoint between the two hydrogens (positive)
    - Charges on atoms: students can determine that oxygen has a negative charge (0.64 e^-) and hydrogens have a positive charge (0.32 e^-), and that the total charge on the water molecule is zero ($0.64 - 0.32 - 0.32 = 0$)

3. What are some of the behaviors of water?

    - Vibrations: when exposed to infrared energy (IR, approximately 700 - 1000 nanometers in length), the water molecule vibrates. Most molecules follow the 3N-6 rule for vibrations, where N is the number of atoms. For water, N=3, so 3(3) - 6 = 3, and we expect to see that water vibrates in three different ways: scissoring, symmetric stretching, and aysmmetric stretching. NOTE: the Wikipedia page on molecular vibrations (`https://en.wikipedia.org/wiki/Molecular_vibration`) has a nice animation of vibration types,The fact that water absorbs and emits IR radiation, resulting in molecular vibrations, is one of the reasons why water is considered to be a greenhouse gas.
    - Molecular density: we typically display molecules using a ball-and-stick model, where the ball is the atom and the stick is the bond (each stick signifies two electrons). Molecules do not, obviously, look like this! If we were to examine a water molecule using something like a scanning electron microscope (SEM), what we would see is a "blob", an electron cloud surrounding the nuclei of the three atoms. This cloud is called an "electron density", and it represents a probability that the electrons are at a specific distance from the three nuclei. We can visualize electron density from performing a molecular orbital (MO) calculation and then looking at the resulting electron density visualization.
    - Electron distribution: water has 10 electrons (eight on oxygen, one each for hydrogen). These electrons are distributed throughout the molecule. If we display an "electrostatic potential" map, we will see that most of the electrons congregate around the oxygen, making this an electron-rich area, signified by a red color on the map. Likewise, few of the electrons are near the hydrogens, making them electron-poor regions, signified by blue. Electron-rich areas are called "nucleophiles", because they are attracted to

nuclei with their positive charge. Likewise, electron-poor areas are called "electrophiles", because they are attracted to electrons in other molecules. So, when water reacts with other molecules, it does so based on the charge distribution on those other molecules.

2 Computational Approach

The graphical user interface (GUI) of WebMO, installed on the server, makes it very easy to build molecules, measure some basic properties, and perform simple calculations, such as finding the dipole moment (in units of Debyes), the electron charges on the individual atoms, the vibrational frequencies, and the electron density and electrostatic potential maps for the molecule.

To learn how to perform these calculations, the reader is directed to this YouTube video: `https://youtu.be/y78WnPactDw`