CALIFORNIA STATE SCIENCE FAIR
2013 PROJECT SUMMARY

Name(s)
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Project Number
S0621

Project Title
Computational Simulation of Multidimensional H(2)O Molecule Interactions

Abstract

Objectives/Goals
This experiment intends to answer the question, #Can the most optimized positioning of water molecules in a multidimensional system, in order to reach the lowest possible system energy, be created by randomly generated simulations?# The hypothesis that the most optimized system can be generated via simulation after initial randomized placement of water molecules will be accepted if the data returned from the program is comparable and realistic data, in comparison to a real system of interacting water molecules. The hypothesis will be rejected if the program is mathematically incapable of producing a system close to minimal system energy. Minimal system energy will be determined by the angle of the individual water molecules and their distances apart from one another. The total energy of the system will then be calculated by taking the summation of the individual iterations of Coulomb Energy between each atom of each water molecule in the system. Coulomb Energy will be calculated through looping processes and dipole moment interaction algorithms.

Methods/Materials
Little physical materials were used in this software-based experiment.
Apple MacBook Pro, Mid 2012, Netbeans IDE, Jmol, Git, Github, & Microsot Excel 2011

Results
By mathematical definition, the closer the molecules, the lower the energy.

Conclusions/Discussion
The program, being able to generate system energies that were close to infinitely approaching zero, shows potential with future versions of this program. The purpose of having a program that can do these water molecule energy calculations will be helpful not only because it is more efficient than when done by the human hand, but also to find answers to questions about different molecular interactions in chemistry. Water molecule optimization can help the world of science better understand how substances dissolve in water, as well as gain a better understanding as to how molecules tightly pack themselves together during the process of freezing. In the future, the program will include things like how systems of water molecules interact with different materials in different situations, like in a zero gravity situation, in a cup, or even on a polar surface like a table. This leads to a new feature of the software that could have the capability of modeling the surface tension.

Summary Statement
Software was written to model three-dimensional water molecule interactions and energy trends.

Help Received
Advisor helped explain math.