CALIFORNIA STATE SCIENCE FAIR
2014 PROJECT SUMMARY

Name(s)

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Project Number

S0619

Project Title

Determination of Accurate Molecular Models of Polyatomic Ions in Aqueous Solutions by Molecular Dynamics Simulations

Abstract

Objectives/Goals

This research wished to develop a theoretical methodology to determine accurate molecular models of polyatomic ions in aqueous solutions. Currently, accurate models of such ions in aqueous models do not exist, but are required to better understand many important environmental effects and to develop efficient industrial and research procedures.

Methods/Materials

Quantum mechanical data and experimental results do not exist for polyatomic ions due to complexity involved in applying current approaches. Hence, we aimed to determine accurate models by correlating values of dynamic simulation-calculated properties with experimentally determined macromolecular properties with values that are well known, most notably solubility. This methodology was conducted and is presented in the context of the polyatomic sulfate anion, SO(4)^(2-). Physical parameters of the ion (bond lengths, bond angles, bonds# spring coefficients, partial charges, etc) were varied and multiple dynamic simulation runs were conducted.

All simulations were started in equilibrium conditions calculated from experimental studies of macromolecular properties of sodium sulfate. If the chosen values of the parameters in our theoretical model were perfectly accurate, the system started in equilibrium should stay in equilibrium and there should be no deviation in macromolecular properties of the simulation space (such as total energy) over time.

Results

During each simulation run, the total energy deviation was determined at regular intervals and was analyzed to calculate the unknown optimal values of the parameters.

Accuracy of these values was validated by running further simulations that used models incorporating the optimal values. Total energy deviation was once again determined and was found to be low. Statistical tests allowed us to conclude that the low deviation was due to the choice of values of the parameters.

Conclusions/Discussion

This novel methodology of correlating dynamic-simulation and experiment determined values of macromolecular properties was proven to find a more accurate model of polyatomic ions in aqueous solutions and is broadly applicable.

Summary Statement

This research developed a theoretical methodology to determine accurate molecular models of polyatomic ions in aqueous solutions, which currently do not exist.

Help Received

Ms. Kavita Gupta (mentor) helped proofread my research paper