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Activity

Computational Chemistry Activities with Avogadro and ORCA

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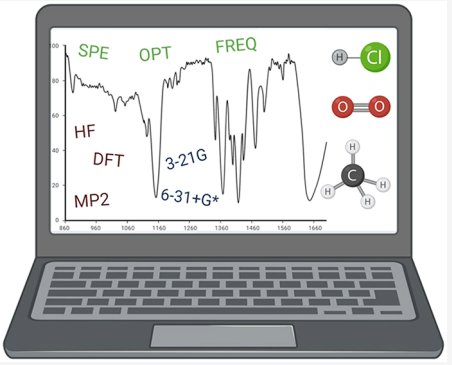
ABSTRACT: Computational chemistry modeling activities that took place as part of a course in physical chemistry are described. The main software tools used by the students were Avogadro and ORCA, which are freely available on the Internet for academic use. Avogadro is molecular visualization software, which can be used not only to prepare input files for a range of computational chemistry software but also to visualize output files from them. ORCA is an ab initio quantum chemistry program containing modern electronic structure methods, such as density functional theory, many-body perturbation, coupled cluster, multireference methods, and semiempirical quantum chemistry methods. Four introductory level computational chemistry activities are described for use in general chemistry and physical chemistry laboratory courses and all are suitable for virtual learning environments. Details of our implementation and the educational value of this work are discussed. In addition, a Student Assessment of their Learning Gains (SALG) survey was conducted after the implementation and the results are reported.



KEYWORDS: *Physical Chemistry, Upper-Division Undergraduate, Laboratory Instruction, Computer-Based Learning, Computational Chemistry*

INTRODUCTION

In recent years, the uses of computational chemistry in the chemistry curriculum has become widespread[1−12] as more and more positive learning outcomes are reported.[13,14] This is significant not only because the simulations can provide valuable insight into chemical behaviors but also computational chemistry provides a hands-on experience of modeling. Modeling, often guided by simplification, can be considered as a visual way of linking theory with reality or the experiment. Model thinking whether the model be philosophical, mechanical or computational, makes students better thinkers.[15,16] Having students understand how models are extensively used in both science research and in communicating science is crucial. They can realize the strategies of computational modeling are somewhat like the strategy followed for the weekly weather forecast: try different models and see how they differ—what is the range of the calculated results? What are probable outcomes? What are the strengths and weaknesses of each model?

As is well-known, models are not perfect. It is not always possible to reproduce experimental results with computation since quantum systems are complex and many measurements reflect the behavior of macroscopic systems that include large numbers of molecules. Even in cases where the model and experiment can be compared and disagree, there may be something new and important to be learned from the disagreement and added to the model. In cases where the model and experiment cannot be compared, one can test hypotheses about basic molecular processes from the model. The direct experience of students with computational chemistry may pay big dividends in enriching their thinking about the scientific process and in creating new ways to understand natural phenomena.

Besides developing models, computational chemistry is a way to experience real life applications of the quantum theory learned in physical chemistry lectures. Traditional introductory quantum mechanics deals with simple systems that illustrate general quantum principles. To the students, it is not obvious how to leap from the simplified analytic solutions of the textbook to more complex phenomena of multielectron atoms or molecules. As is well-known, beyond the simplest cases, analytical solutions do not exist. The nucleus and its electrons are a dynamic, many-body problem that has no closed-form solution. To make the connection between analytic solutions of a student's textbook and computational chemistry results, we provide an interactive html/javascript Web site (https://quantum-wave.s3.amazonaws.com/wave1d.html) that allows students to explore how energy levels are found numerically using Schrodinger's equation in manual steps. Three simple, symmetric systems are available: particle-in-a-box, harmonic oscillator and quartic oscillator. The program graphs 5

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solutions to Schrodinger's equation, equally spaced over an energy range and students find the allowed energy levels by bracketing solutions that go to zero outside the potential boundaries. Students also measure wave function wavelengths and test if Heisenberg's uncertainty principle is satisfied. The solutions to the particle-in-a-box are compared to an analytic solution. An investigations guide and solutions to the investigations are posted in the Supporting Information.

To deal with complex molecules, the best one can do is to utilize an ab initio quantum chemistry program that includes modern electronic structure methods. Using iterative, computationally intense methods, problems may be solved by computational chemistry models. These models try to balance accuracy with efficiency. An advantage of this approach is that it opens up a broad range of applications to trials and studies of structure and interactions. One disadvantage of this approach is that the computer software is somewhat of a "black box" to students who use it. In science and our laboratories, we use magic "black boxes" all the time. You learn what inputs to provide and how to interpret outputs. For software as well as other applications, what counts is how much you know about your tool or instrument? Do you use it blindly or guided by reasoned judgments? Do you know its strengths and weaknesses?

To offset this "black box" disadvantage, one can discuss with students the strategies and methods used by the computational software to develop solutions and make clear that the quantum rules and laws of the textbook are applied numerically in an approximate form to complex molecules.

In our course, two laboratory periods in physical chemistry were devoted to a basic introduction to computational quantum chemistry principles and a review of different methods including Hartree−Fock (HF), Density Functional Theory (DFT) and Møller−Plesset perturbation theory (MP2).

The first week, after a general introduction about simulations and modeling, the Schrodinger equation was reviewed, and then, the Born−Oppenheimer approximation was introduced. Focusing on the electronic Schrodinger equation, potential energy surfaces and electronic properties such as dipole moment, polarizability, vibrational, rotational, IR and NMR spectra can be obtained. After that, HF was introduced. The electronic wave function was written as an antisymmetric product of molecular orbitals, MOs, (a Slater Determinant), in which each electron feels only the electric field of an average charge distribution due to other electrons. At this point, we discussed how models use approximations to get results and that this use of an average charge distributions is an approximation. Then, the HF wave function and the method of expressing each MO as linear combination of atomic orbitals (AO) were discussed. The iterative nature of finding the HF function was presented as was the method of finding the orbitals (coefficients) by minimizing the HF energy, which, itself, is a function of the orbitals. The solution method starts with a guess and solves iteratively (the self-consistent field model). This first week's lab period also included basic molecule building and discussion of functions of the Avogadro software.

The second lab period involved an introduction to ORCA and the command line user interface with basic commands. The discussion from the previous week was continued by introducing basis sets and by answering the important question: How do we pick AOs? MOs are commonly constructed from AOs. Details of basis sets were presented, and the students were referred to the accuracy discussion of the ORCA basis sets[17] for an in-depth explanation of how they affect the accuracy of predictions. After that, MP2 was discussed, starting with the approximations made in HF and then detailing how MP2 treats electron correlation explicitly (more accurately and costly) as a "small" perturbation to the HF method. Configuration interaction and coupled cluster methods were also briefly introduced as more accurate but more costly methods. Finally, density functional theory was introduced as a model in which many-electron wave functions were replaced with electron density functions and the energy is minimized with respect to electron density instead of atomic positions. The discussion was concluded by comparison of various methods and applications of computational chemistry.

In their work, students were then left to form judgments, based on their trials and knowledge of electronic structure theory, how accurate their software "tool" might be. We stressed that models are an approximation with a great potential to accurately simulate molecular structure and behavior.

The computational chemistry software is more than an educational "toy". It represents a class of computational tool that is state-of-the-art and used for authentic research. As such, we should want to train students in use of the tools. Training is necessary so that students do not just accept any result computed by the software; some knowledge, judgment and trials are sometimes needed to sort out facts. By applying several different methods on the same problem, students can see how they differ and they can review the theory on whether these differences are expected.

In this article, we describe our own implementation of computational quantum chemistry exercises during weekly 3 h Physical Chemistry lab periods in Fall 2017 and Fall 2019. While the lecture class covered topics of quantum mechanics and spectroscopy, students in the laboratory practiced the application of quantum mechanics to molecular models. The computational exercises and use of software were new (as far as we knew) to all the participating students. So, the work was kept at a basic, introductory level. We focused on having the students practice a pattern of behaviors that would serve them in their future work with computational chemistry or with any simulated models.

Students of the 2019 lab were given a short survey after all the laboratories were completed to track their response to the new computer instruction. The number of students was small ($N = 8$), so the statistical significance of trends and results is limited. The survey questions focused on gains in student skills and in their attitude about physical and computational chemistry. Most students reported moderate to great gain. The student lab reports provide a measure of student comprehension.

BACKGROUND

Gallaudet University is a small liberal arts college for deaf and hard-of-hearing students. The university offers BA/BS degrees in chemistry. The school year is divided into two 14 week-long semesters.

The main software products used by the students in the Fall 2017 and 2019 laboratories were the molecular editor Avogadro[18,19] and the quantum chemistry software ORCA.[20] Both are freely available for academic use. Avogadro provides an intuitive, interactive interface for constructing molecular

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Table 1. List of Computational Activities Utilized (See SI)

	Lab Exercises	Details
1	Computational prediction of molecular structures of selected small molecules	Basic introduction to computational chemistry and reinforcing learning about VSPER theory. This was included in our general chemistry curriculum.
2	Determining optimized structures for selected molecules	This experiment is an introduction to computational chemistry and involves optimization calculations of several small molecules at different levels of theory. Instructions also include single point energy calculations on distorted molecular structures to indicate structure(stability)-energy relationships.
3	Vibrational spectroscopy calculations of HCl	This activity is a complementary experiment for the traditional infrared spectrum of HCl experiment. Students obtained IR spectra of HCl at different levels of theory and compared each with the experimental spectrum to gain insights on how the results compared.
4	Morse potential or harmonic oscillator	In this activity, students were asked to do single point energy calculations at different H−Cl distances from 0.1 Angstrom to 2.5 Angstrom with 0.1 Angstrom increments. Then, they were asked to fit the data to Morse and harmonic oscillator potential equations and decide which one is a better approximation for modeling HCl bond vibration behavior.

models and for visualization of molecular structures and spectra. ORCA provides electronic structure calculations. Avogadro provides a visual way to prepare ORCA input files and to visualize output ORCA files.

Computers running Windows 10 (64-bit, Intel Core i3-i7 CPU at 2.4−3.4 GHz with RAMs 8−16 GB) were available for student use in a campus laboratory. No problems were encountered with installation of both software products on Mac, Windows 7 and 10 computers.

We have mentioned that the undergraduates at our school are deaf or hard-of-hearing. For deaf students, as well as others, three-dimensional modeling programs like Avogadro improve greatly on the traditional molecular symbolism of ball-and-stick models, textbook two-dimensional sketches or algebra-like equations. These traditional representations do not capture essential three-dimensional features that are important for predicting interactions.

Visualization of the structure of molecules, the geometric arrangement of their atoms and their electron density clouds, is important for study of molecular interaction and bonding characteristics. Computer graphics provides an easy-to-use tool for constructing and manipulating three-dimensional objects. Beyond basic 3-D visualization functions, the computational chemistry software calculates accurate molecular structures and spectra based on quantum laws with various approximations. This is the important educational leap where students see the impact of the physical laws constraining their 3-D molecular "artwork".

Visualization and imagery help students to understand content and the importance of visualization in science courses has been well established.[14,21] In the case of deaf students, visualization and manipulation might be very important for learning. In general, deaf students have historically faced challenges in achieving the same level of reading comprehension as their hearing peers.[22,23] One way to improve reading comprehension is through imagery.[23−25] Prior experiences with visualization imagery was found to promote reading comprehension skills in deaf students[26] and adults.[27]

One might judge that similar conclusions could be drawn about visualizations being helpful for ESL (English-as-a-Second-Language) learners, as well as other students. The reading of science texts can be challenging in cases where the understanding of content is not reinforced by some form of prior experience and mental imagery. Computer visualization with manipulation tools provides a realistic "interactive" environment for productive, creative modeling and investigation. This type of activity has a potential to stimulate the imagination, promote informed intuition, and develop more scientifically based thought processes.

In addition, deaf or hearing ASL (American Sign Language) users were found to have an enhanced ability to generate mental images and detect mirror reversals.[28] This is possibly due to visual nature of American Sign Language, ASL, and its specific linguistic requirements including referent visualization, topological classifiers, perspective shift, and reversals during sign perception.[28] Research has also found that deaf ASL users more quickly generate visual mental images compared to hearing nonsigners, which was attributed to strong right hemisphere advantage for image generation in signer deaf brains.[29] Therefore, one might expect that including visualization might enhance signing students' comprehension more so than nonsigners. This is an interesting area open to further investigation. We would like to emphasize that the computational activities described here is suitable for any student and not specifically designed for signing students.

METHODS AND COURSE PLAN

Guides for the computational chemistry exercises (Supporting Information) were prepared and made available to students. Initial activities included necessary prelaboratory tutorial activities (Avogadro tutorials)[30] and an introduction to command line instructions[31] to help students become accustomed to the software. Online tutorials were provided as part of the Avogadro documentation.

As described in the introduction, prior to the computational chemistry activities, the relevant computational quantum chemistry theory was covered in the lab including Hartree−Fock, Møller−Plesset Perturbation Theory, Density Functional Theory, basis sets, and several applications. It was left to students' observations, research and judgment about how these methods compared in regard to accuracy and efficiency. After this general introduction of the theory, each lab session started with a brief demonstration of any new computer skills and a discussion about the specific computational chemistry focus. Students, then, began their work, constructing molecules and extracting data.

There were several goals of the computational chemistry activities:

1. Integrate use of computational chemistry software into a physical chemistry laboratory course.
2. Train students to follow a learning-research pattern of behavior: learn necessary computer processing techniques, do computations, extract information, organize data, and research/derive conclusions.
3. Provide experience to students constructing molecules using various geometries and reveal the effects of optimization and how it is related to the potential energy and stability.

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J. Chem. Educ. 2021, 98, 1335−1341

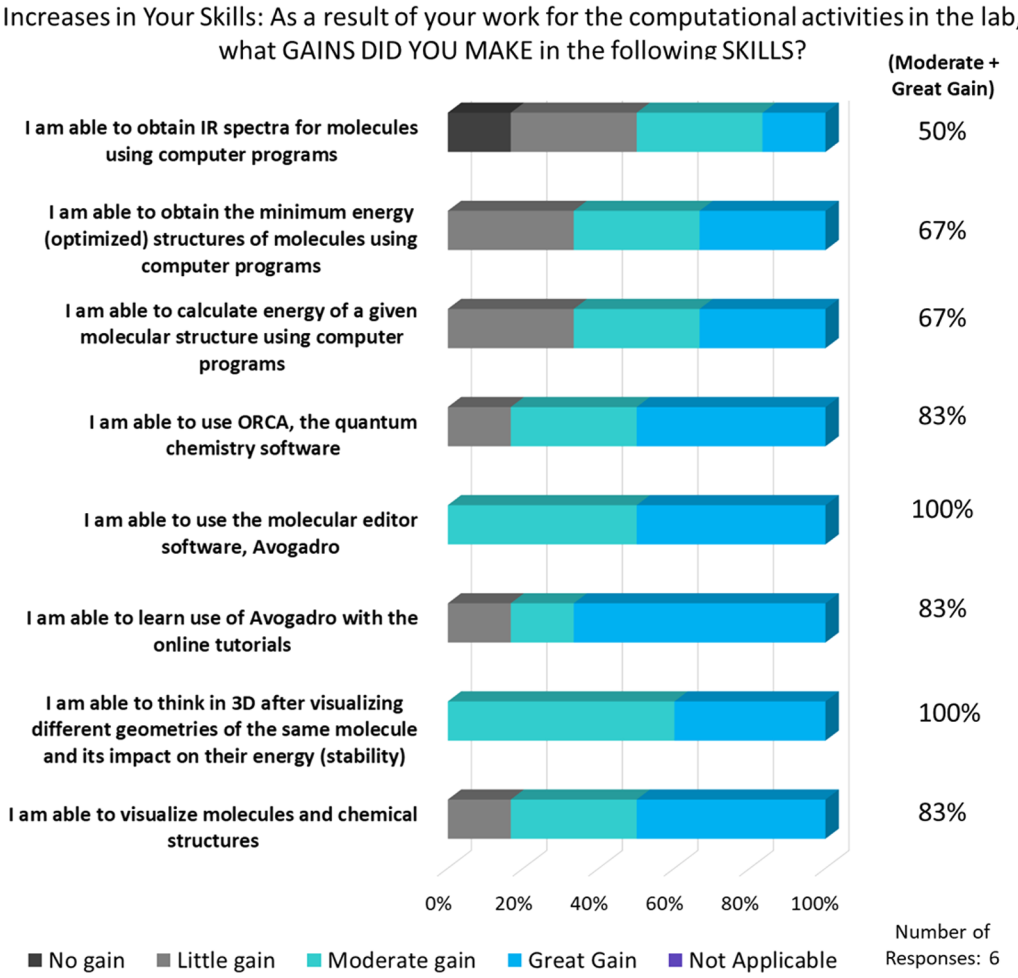

Figure 1. Student responses to the first part of the SALG survey.

4. Show how modeling works in real life through comparison of computed and measured parameters.

The four lab exercises described in Table 1 are provided as a Supporting Information (SI) to this paper. One of them (#1) is being utilized in our general chemistry laboratories and the other three (#2−4) in the physical chemistry laboratories.

Students had little trouble with the Avogadro software. The online tutorials for Avogadro were clear and worked well as prelaboratory activities. Avogadro has a windows GUI (graphical user interface) that most students recognize from their use of computers. ORCA, on the other hand, uses a command-line interface (CMD). Unlike a GUI, which restricts the command options, the command line interface responds to whatever command is typed, and it can be very powerful, especially for automating routine tasks. Students were taught basic file execution and manipulation commands to use in the terminal window. ORCA reads text input files and produces text output files. The outputs from ORCA were visualized using Avogadro with no problem. After some practice, students seemed confident about using both Avogadro and ORCA.

■ ASSESSMENT AND DISCUSSION

At the end of the Fall 2019 laboratory course, an online Student Assessment of their Learning Gains (SALG) survey was sent to students. The first part of the SALG survey was aimed to measure student perceptions on how their relevant skills were impacted by the computational activities utilized in the lab. The second part aimed to measure how students perceived their own learning of the content and their attitude toward the topics covered and the course. In the online version of the survey, students were to choose one of the six options (from No Gains to Not Applicable (Figure 1)) for each item. Figures 1 and 2 show the two main survey questions, prompts and responses. Six out of 8 students filled out the survey. As mentioned before, this limits the significance of conclusions drawn from the survey.

As can be seen from Figure 1, students felt confident in their abilities in using Avogadro and ORCA programs as all students (100%) stated that they are able to use Avogadro and 83% stated that they are able to use ORCA (moderate plus great gain). Although the options utilized in ORCA were kept at an introductory level, one student perceived it as difficult to use which can be attributed to the fact that this was the first time students were exposed to a command line-based program (ORCA) without a visual component. We foresaw this difficulty and, therefore, introduced CMD instructions in previous lab periods when discussion computational chemistry concepts. However, that introduction did not involve any follow up assignment. To avoid any difficulty due to lack of familiarity with the CMD interface, it would be good to practice use of file manipulation commands (executing, moving, copying, editing, deleting, making directories). Except for one student, Avogadro's online tutorials were found to be sufficient to learn how to use it.

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J. Chem. Educ. 2021, 98, 1335−1341

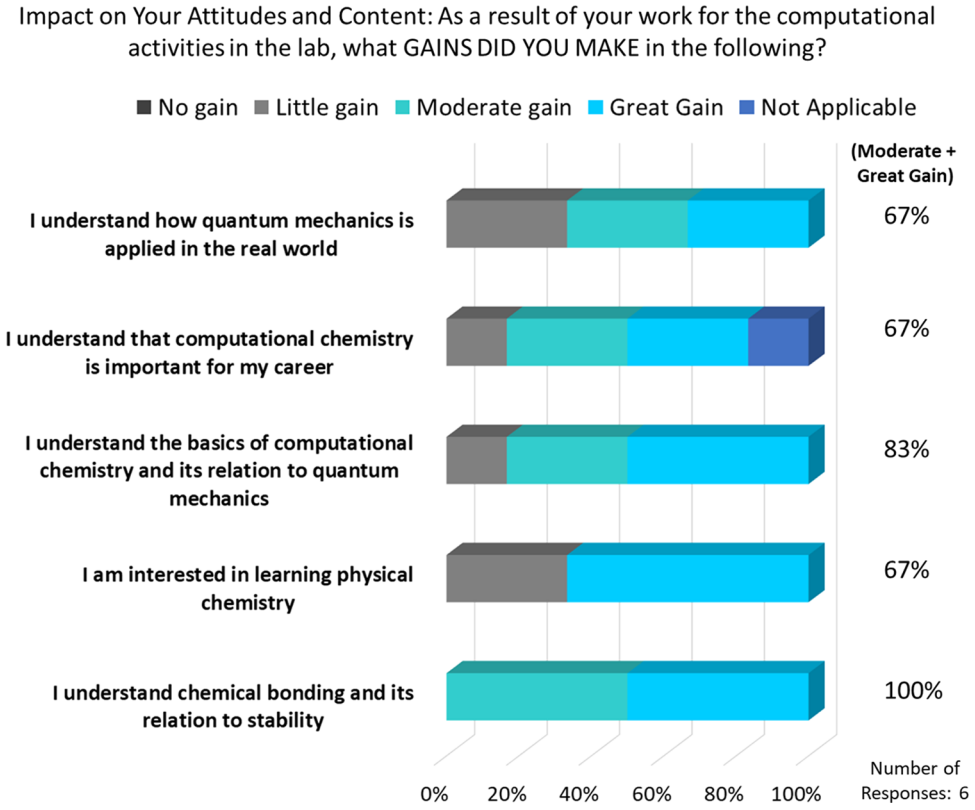

Figure 2. Student responses to the second part of the SALG survey.

Regarding visualization of molecular structures, all students except one felt that the computational activities resulted in great or moderate gain in their ability to visualize molecules and chemical structures. In addition, 100% of students indicated that there was a moderate or great gain in their ability to think in 3-D to visualize different geometries of the same molecule and to see how the geometry affects its stability. During the computational activities, the relation between structure, energy and stability were discussed several times particularly during the optimization activity (activity #2). The student lab reports provided an indication of student comprehension. In their reports, all students except one discussed the relationship between the structure and potential energy. One student elaborated on this and explained some aspects of the theory. She also discussed basis sets and some details of MP and DFT along with comparison of her results in regard to accuracy indicating a sufficient basic understanding of the theory.

Concerning how students perceived the increase in their skills in calculating energies of molecules and in obtaining optimized structures and IR spectra, students reported the least gain (50% for moderate or great gain). The keywords in Avogadro for preparing ORCA inputs for each of these tasks are stated as "single point energy", "optimization", and "vibrational frequency" as is common in nearly all computational chemistry software. All that needed to be done to calculate these is to pick the keyword in a tab provided in Avogadro. Students started using the single point energy and, then, moved onto optimization and vibrational frequency jobs. We suspect that some students might not have made the connection between the "vibrational frequency" and IR spectra. This might be because the follow up work (lab report) for the IR spectra involved more complicated calculations compared to others, therefore students might have perceived less gain in pursuing the IR spectra calculations.

Although all computational chemistry exercises used in this laboratory section involved comparison of different levels of theory with the experimental structure (or comparison of two models as in the case of Morse potential versus harmonic oscillator), our SALG assessment did not adequately survey perceptions about these issues. Not only did the activities involve these comparisons but also the strengths and weakness of different levels of theory were discussed in the laboratory prelab and postlab sessions. It would have been useful to see how students perceived their gains in model thinking. We plan to add questions related to models thinking next time when these activities are utilized. Review and analysis of student reports indicates that all students except one discussed models and approximations at least at the very basic level, while two students elaborated on that topic, giving some other examples of using models.

Figure 2 shows the results of the second part of the SALG survey. All students reported that they are able to see the connection between chemical bonding and stability as a result of the computational activities, which is consistent with the results reported in the first part of the SALG survey. Except for one student, all students reported moderate or great gain in their understanding of computational chemistry and its relation to quantum chemistry. On the other hand, only 67% reported that they had a moderate or great gain in understanding how quantum chemistry applied in the real world. This is a surprising result for us since we expected that these activities would in fact be perceived as a great way to demonstrate the application of quantum mechanics in real world. One way to overcome this could be an experiment design lab in which students may choose a system of interest and use the methods

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J. Chem. Educ. 2021, 98, 1335−1341

that they previously learned to study this system. This activity can be added without using an additional lab period. A sample rubric that can be used for such activity is included in the SI. Another way to strengthen the real-life connection would be implementing the computational experiment on single-walled carbon nanotubes (CNTs) by Simpson et al.[11] Students can prepare the systems using the nanotube builder extension implemented in Avogadro and perform the calculations in ORCA.

Lastly, 67% of students reported a moderate or great gain in how they perceive computational chemistry in their careers or their interest in learning physical chemistry. This is a great gain because an informal discussion at the beginning of the class showed that all students were taking physical chemistry only to meet their degree requirements.

CONCLUSION

Overall, the students worked well with the software and seemed to grasp the main ideas raised in the lab guides. Since both Avogadro and ORCA were freely available for academic use, students were able to download them into their laptops and use them without license issues. In addition, students were able to use online manuals with no problem. Our main goals for introducing computational chemistry into physical chemistry I included accustomizing students to model thinking and providing real life applications of quantum chemistry.

The SALG survey filled out by students at the end provided insights on how students perceived their gains in skills and some topics as well as attitudes toward physical chemistry and computational chemistry. Overall, most students reported moderate or great gain in all areas covered in the survey.

We are working toward integrating computational chemistry into chemistry curriculum from general chemistry to all our major chemistry courses. As mentioned earlier, exercise 1 of Table 1 (SI) is in use for our general chemistry laboratory and exercises 2−4 (SI) are used in physical chemistry I laboratory. Currently, we are developing exercises for our organic chemistry courses utilizing Avogadro and ORCA.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.0c00959.

Wave 1d activity (PDF)

Computational prediction of molecular structures of selected small molecules (PDF)

Determining optimized structures for selected molecules (PDF)

Vibrational spectroscopy calculations of HCl (PDF)

Morse potential or harmonic oscillator (PDF)

Experiment design sample rubric (PDF)

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Notes

The authors declare no competing financial interest.

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