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Teaching and learning of chemistry with computers

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Abstract

As the new generation of students who are savvy with technologies and computers, along with the developments in computer hardware and software, the learning curve of computational chemistry is weakening. We establish various modules that can be used not only to demonstrate the challenging concepts in chemistry education, but it also provides the pro-activeexperience that allow students to generate their own data and conclusions.

Keywords: computational chemistry, molecular modeling, undergraduate chemistry, chemical society

1. Introduction

The new generation of students is totally different from the generation we used to teach [1]. This generation wants to learn things in a different and quick way, and they seem to be less patient to read books, though we believed that's the only way to learn the new information. Some of them will never open their books before the exams, sometimes not even before the end of semester. They search answers and concepts on Google, irrespective of the accuracy and correctness of the answer. The problem occurs when some of these students would simply copy and paste online answers and claim their credit, which we call plagiarism. Chemistry is also similar to other science subjects that are facing this problem.

According to a survey conducted in 1995 [2], many students describe chemistry as one of the toughest and most boring science courses they must pass, despite the fact that chemistry, a science central to technology and engineering fields in many ways, is an easy subject to apply to real life [3]. The examples and applications of chemistry are plentiful and inevitable in everyday life. For example, an understanding of fundamental chemistry concepts are required to solve the ongoing energy crisis, to develop environmentally friendly methods of production and waste management, to develop better medicinal drugs, to solve environmental problems, and to design newer functional nano-materials. Therefore, chemistry along with other science courses such as physics and math usually are weaved into the university core courses that almost all incoming freshmen will have to take and pass. Depending on the major and classifications, most campuses will have a chemistry course for students majoring in non-science related subjects such as nursing, technology or engineering [4] and there are separate courses set up just for the chemistry, biology, and other science majors. These chemistry courses require a significant amount of foundational knowledge of electronic structures, electron configurations. After they've learned these basic fundamentals, we then demand the student to apply and correlate between the structure and property, and finally predict the properties of new materials. The job market demands our students to at least have some type of exposure. For example, the foundation-level chemistry curriculum should be reorganized into three sequences: structure, reactivity, and quantization. It is believed that the new reorganization would allow students to more quickly appreciate the breadth of the field than the traditional domains. With the dilemmas and the new challenge brought upon us by this new generation of learners, they have also brought new opportunities. For example, most of them now have tons of electronic gadgets at their disposal and most of time they are online for social or entertainment purposes. There have been some researchers and educators who embrace electronic teaching such as distance learning, podcast, mini-video streaming, along with clickers, traditional power points, and transparencies. In this paper we will explore computational chemistry, In particular the molecular modeling tools that are used to

1. Help students understand difficult concepts such as electron configuration and structural modification, in general chemistry setting, and
2. As a research tool for advanced chemistry courses or scientific research.

2. Approaches

There are two different types of students who take chemistry: the science majors and non-science majors. In general, the science majors usually find it easier and would adapt to, if not already being trained on, the traditional conceptual approach of learning chemistry, which often is taught in the form of rigorous facts and principles and very much in an abstract manner. On the other hand, the non-science majors are still in need of developing some types of scientific (aka chemical) literacy, which would then allow them to understand the principles, and engage in an interactive way to grasp the materials and possibly apply those principles to better understand the phenomenon around them from environmental effects to nanotechnology [5]. It is not surprise that the non-science majors find this traditional approach to chemical education difficult and boring, and are struggling to understand the relevance of conceptual chemistry. Most of these students will lose their interests in science, particularly in chemistry within the first year because of the embedded requirement in core curriculum.

3. Methodology

In this study, we will use computational technology to expound upon various chemistry situations. As examples, we will use it to describe the kinetics of substitution reactions. Finally, we will describe how computational chemistry can be used not just in the methods listed above but in other aspects of chemistry. By using this tactic, it allows students to produce the data quickly and draw their own conclusions as they learn from the textbook.

4. Results and discussion

One of the important and vital tasks as a chemistry educator is how to move away from the perception that chemistry is difficult and boring. This perception was developed during the early stage of Chemistry and physics around 1920s when more fundamental discoveries helped form the theoretical principles. These discoveries allowed chemistry to become more rigorous and analytical, which also made the field highly submerged in tradition [6]. As such, the material that needed to be covered in general chemistry exploded over the years. To make things worse, the new materials were simply augmented and added without evaluating their relationship to old principles. A review by Lloyd in 1992 pointed out that the typical general chemistry textbook changed from a small 5 inch x 8 inch book into a 1000+ page, 8 inch x 10 inch encyclopedia book that averaged 6 lbs [7].

Clearly there is a need to modernize how chemistry is taught to our new generation of students. There are many published efforts and research that has been invested in endeavors to assist students' learning, such as MIT's Open Course Ware [8], and Peer-led Team Learning (PLTL) [10]. As their names suggest, all these approaches actively involve the students either on problem-based or real life scenario-based self-instruction and self-teaching. The results would have been somewhat successful if the approach was well planned and implemented. While our approach in this study also adopted student-centered engagement, we employed computational chemistry and molecular modeling as a tool to facilitate the student learning.

The computer technology and software development has enabled modeling tools to be used on a par with experimental methods as a legitimate and practical means for exploring chemistry. Molecular modeling can offer major benefits as a tool for exploration such as studying a compound that is difficult to synthesize in a laboratory setting. The cost of making this compound on screen is essentially just the price of the software itself and the creator's imagination. However, one must be very cautious of such actions as the traditional wisdom says "Garbage in, garbage out." Therefore, the guidance from a more experienced user and instructor is essential in teaching the "right" chemistry. That way, students will not be taught improperly. Compared to the cost of synthesis, purification and characterization costs, modeling tools provide crucial information on geometries, 3-D rendering, volumes, contact areas, symmetries, reaction mechanisms, and energy profiles such as activation energies for kinetics and thermodynamic parameters such as enthalpy, entropy and Gibbs free energies.

Like any discipline, good science instruction should start with well drafted learning objectives and learning outcomes as one of the essential tools for the success of the course and a guide for students' learning. Literatures show that learning objectives and learning outcomes follow more than two dozen taxonomies that have been developed to define the domains of learning, development, and cognition [11]. However, most of them were all based on Bloom's classic Taxonomy developed in 1956 [12] as shown in Fig. 1. While Bloom's classic Taxonomy of Educational Objectives were defined by six hierarchical levels of cognitive processing, (knowledge, understand, apply, analyze, synthesize and create), a more modern version of Bloom's Taxonomy use a non-hierarchical definition of learning (knowledge, comprehension, application, analysis, synthesis, and evaluation) [9].

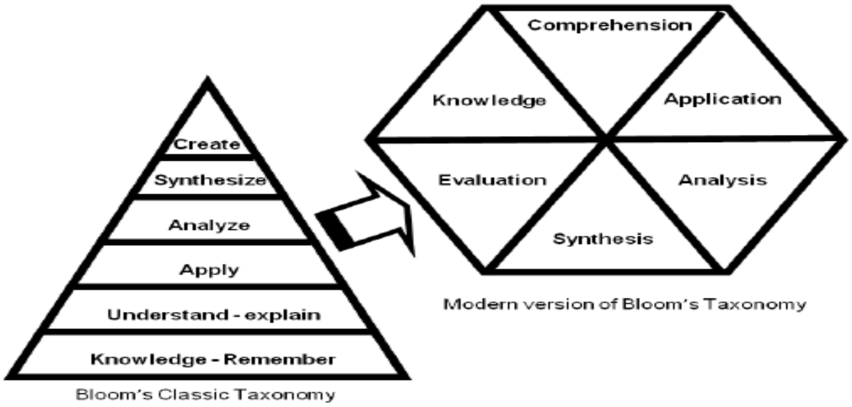

Fig. 1. Bloom's classic Taxonomy developed in 1956.

Though the words of these versions are similar, the approach to assist students' learning is quite different. The classic hierarchical approach assumes students' progress gradually from bottom up, while the non-hierarchical approach assumes students' learning at all levels and all aspects. These different learning skills were developed concurrently, therefore training of these skills need to be applied correspondingly. There are even other types of taxonomy such as foundational knowledge, application, integration, human dimension, caring and learning how to learn. Computational chemistry and modeling tools actually enable students to apply, analyze and synthesize the chemical concepts embedded in the question through the data generating, collecting, and analyzing. Here, we will demonstrate some of the modeling modules adopted and developed to illustrate how computational chemistry can effectively explain and visualize the difficult and abstract chemical concepts.

Kinetics of Bi-molecular Substitution Reactions

The reaction pathway and its theories are something that is usually demonstrated via diagrams such as Fig. 2.

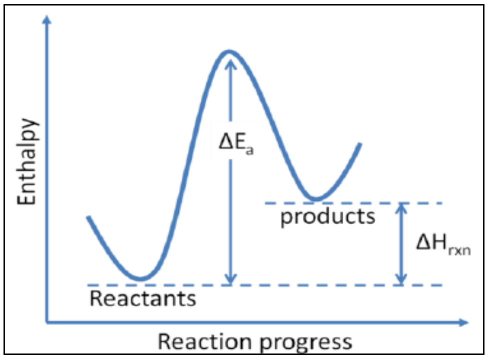

Fig 2: The energy diagram of a reaction coordinate for a simple one-step reaction.

According to the collision and transition state theory, the reactant molecules must effectively collide (geometry-wise and energy-wise) in order for the reactants to enter a transition state (TS) before they can form the products. This collision effectiveness is the key to the activation energy as depicted as ΔEain Fig. 2, which is the minimum energy that must be supplied by the collisions in order for a reaction to occur. The energy difference between the reactants and products determines the endothermic or exothermic energy of the reaction (See Fig. 3). Students have a hard time picturing the transition states and the collision. Therefore, a carefully designed reaction such as a one-step nucleophilic substitution reaction (SN2) of bromide with methyl chloride, could be used to illustrate the concepts. The steps implemented are:

1. Prepare the reactants CH3Br+Cl- and the products CH3Cl+ Br-
2. By fixing C-Br bond, scan the bond distance between C-Cl from 1.7 to 4.0 A
3. Swap Br-Cl position, then fix C-Cl bond distance to the lowest energy point in above scan, scan the C-Br bond distance from 1.7-4.0 A.
4. Deduce the possible geometry of transition state based on above steps
5. Use Scan function of Gaussian to set up automatic 2-Dscan of C-Cl and C-Br distance and plot the geometry of transition state to be compared with the results above steps
6. Plot the relative energy of the reactants CH3Br + Cl- the products CH3Cl + Br-, and transition state

This process actually can be used to serve three folds of teaching: *first*, to provide a visualization of the geometries of reactants, products and especially the transition state motion. For example, the frequency of the transition state can yield the concerted motion of leaving group and entering group, such motion is extremely valuable to demonstrate TS.

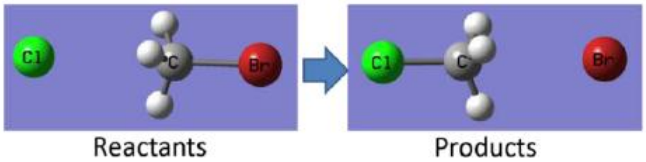

Fig. 3: Visualization of the reactants and products.

Second, providing the understand of the relationship among the Lewis dot structure, electro negativities of Br and Cl, geometry and dipole moments. As shown below in Table1, the calculated geometric parameters are carbon-halide bond distance (Å), dipole moment (Debye), and atomic polar tensors charge and population analysis (e-). Students can easily draw the correlation between these calculated parameters to the electro negativities and geometries of reactants and products. While the explanation provided by most textbooks is readily available, this process allows students to produce the quality data, formulate and synthesize their own conclusions.

Table 1: The calculated parameters of reactant and product Electronegativity dipole C-X bond Charge on X

CH3Br	2.93	2.122 2.009Å	-0.227
CH3Cl	3.122.457	1.867Å	-0.065

Third, students can then search and deduce the TS geometry using steps 2 and 3, while the software generates and pinpoints the TS on the potential energy surface (PES) of reaction pathway in step 5. A PES scan along C-Br and C-Cl bond direction provides students the approximate location of the transition state as shown in Fig. 4. This process could allow students to see the principle and foundations behind the software in search of the transition state as well how the software identifies and evaluates the kinetics of a reaction.

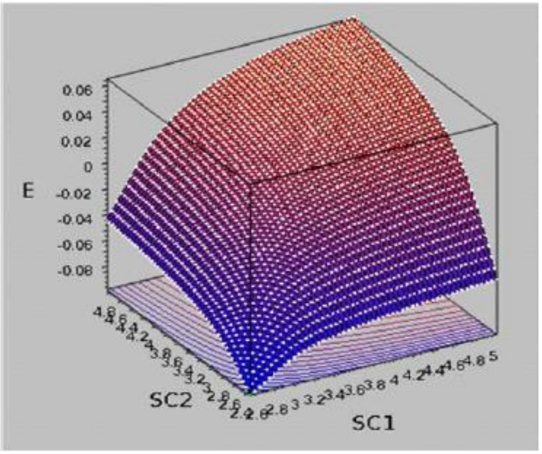

Fig 3

Other Modules

There are many online resources such as a tutorial for the software available for computational chemistry and molecular modeling in chemistry instruction. Especially inorganic and physical chemistry, there are many examples in the textbook can be modeled and compared. Table II lists the example list of modules developed.

Table 2: The example list of modules developed

Title	Concepts explained
Identify isomer equilibrium	Chirality and R/S designation, Equilibrium constant,
Comparison between Benzeneand 1,3,5-cyclohexatriene	Enthalpy, resonance stabilization, enthalpy of formation, delocalization effect
Vibrational analysis of functional groups	Infrared spectra, electron donating and electron withdrawing groups
Rotational barrier investigation	Resonance structure, delocalization of π-bond, effective barrier
Polarities of molecules	Dipole moments, Lewis dot structure, VSEPR model, electronegativity

5. Conclusions

Computational chemistry and molecular modeling tools are becoming available and accessible to students. The calculation ability also becomes more and more powerful due to advancements made in the hardware design and software development. In this study we demonstrated various approaches that can be utilized to exemplify the difficult concepts found within the chemistry education, affording the students the necessary hands-on experiences that are essential in allowing them to generate their own opinion and conclusions.

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