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# Promoting Significant Learning: A Case Study in Computational Chemistry

Ruben D. Parra, DePaul University, rparra1@depaul.edu

Abstract. This paper describes pedagogical efforts implemented to promote significant learning in a computational chemistry course. The taxonomy of significant learning advanced by Fink (2013) is used as a framework to discuss the results. Fink identifies six categories of learning: foundational, application, integration, human dimension, caring, and learning how to learn. Significant learning occurs when all six kinds of learning are promoted. In the computational chemistry course, the learning outcomes are aligned with these kinds of learning, and students are provided with learning activities to get them engaged with the course content. These activities purposefully activate students' prior knowledge, increase their motivation, develop basic skills, apply and integrate what they learn in realistic situations, develop an appreciation for computational chemistry as an ally in science, and further their ability to work independently and with others, and to continue learning about the subject matter beyond the course.

Keywords: Effective teaching, computational chemistry, course design, significant learning

The concept of learning is a complex one as seen by the many proposed definitions and learning theories. Learning theories serve as frameworks for research in education (Lederman & Lederman, 2015). Some definitions of learning refer to gaining knowledge and expertise (Knowles, 2012), while others emphasize changes in attitudes and dispositions. In particular, Reif (2008) considers that upon learning the learner can do things he/she could not do before. Defining learning is important in the context of teaching as intentional support to facilitate learning. These notions about teaching and learning appear supported by research on how learning works (Ambrose et al., 2010) and on how people learn (Bransford et al., 1999). Davis & Arend (2013) correlate teaching success with learning, implying the need to identify and facilitate ways of learning that best matches the intended learning. Biggs (2003) underscores the need for developing instructional strategies that increase the level of students' engagement in deep learning. According to Biggs, deep learning is revealed in the ability to build new knowledge from previous knowledge. In contrast, surface learning relies on accumulating ideas as isolated and unconnected items. Fink (2013) also understands learning in terms of change, and submits that the change experienced by the learner has to be worthwhile. Therefore, quality learning should correlate with the amount of effort that goes into teaching and the effort put by the learner during the learning process. When the change experienced by the learner as a result of instruction is lasting and important in the learner's life, Fink deemed the change as *significant learning*. Thus, it seems appropriate to infer that "*effective teaching leads to significant and lasting learning*". This definition entails the challenge of designing and implementing significant learning experiences. To help meet this challenge, Fink developed a taxonomy of learning and called it "Taxonomy of Significant Learning". This taxonomy was proposed as a successor of the well-known Bloom's taxonomy of the cognitive domain (Bloom, 1956). In its original form, Bloom's taxonomy included six levels: *Knowledge*, *Comprehension*, *Application*, *Analysis*, *Synthesis*, and *Evaluation*. The taxonomy is hierarchical in nature with the first three categories listed representing lower levels of cognition, while the others representing higher-order levels. Since the publication of Bloom's taxonomy, other learning taxonomies have been proposed. Anderson et al. (2001) proposed a version of Bloom's taxonomy wherein the hierarchical nature of the original version remains but three categories are renamed and all categories are expressed as verbs. One important aspect of this revised version is that the authors explicitly consider how the taxonomy interconnects with and acts on different levels of knowledge: *Factual*, *Conceptual*, *Procedural*, and *Metacognitive*. An alternative to Bloom's taxonomy is the SOLO taxonomy (Structure of Observed Learning Outcomes) that serves as a framework to examine the extent and quality of learning at the surface, deep, and conceptual levels on a scale of five levels of increasing sophistication (Biggs & Collis, 1982). In contrast to Bloom's taxonomy, the SOLO taxonomy provides a useful guide for establishing criteria for both writing and evaluating learning outcomes based on the desired levels of understanding (Biggs, 2003). Marzano's taxonomy is yet another alternative to Bloom's taxonomy that provides a framework for distinguishing higher from low-order thinking (Marzano & Kendall, 2007). In addition to the cognitive domain, Marzano's taxonomy emphasizes both the metacognitive and the self-system. The metacognitive system involves monitoring the learner's own process, while the self-system addresses the emotional response to learning.

In contrast to the hierarchical nature of the learning taxonomies described previously, Fink's taxonomy is relational and synergistic. Here, six categories of learning are identified: *Foundational Knowledge, Application, Integration, Human Dimension, Caring,* and *Learning How to Learn*. The nature of these categories ensures that promoting one type of learning increases the likelihood of success in achieving the other kinds of learning. Fink's taxonomy extends beyond the cognitive domain to include aspects of the affective domain like human dimension and caring. A brief description, taken from Fink (2013), of the six categories is presented below.

*Foundational Knowledge*: Acquiring basic understanding of basic data, concepts, relationship, and perspectives as well as the ability to recall this knowledge in the future.

*Application*: Using foundational knowledge. It includes developing particular skills, learning how to manage complex projects, and developing the ability to engage in various kinds of projects.

*Integration*: Connecting and relating various things to each other.

*Human Dimension*: Learning about oneself and others. It involves addressing the important relationships and interactions we have with ourselves and others.

*Caring*: Developing new feelings, interests, and values. It involves caring more deeply about something.

*Learning How to Learn*: Becoming a better learner. It implies developing the ability to inquire about a subject to construct and expand knowledge, and the ability to monitor and regulate own learning.

According to Fink, "truly" *significant learning* is expected to take place when all six learning categories are promoted. The taxonomy of significant learning appears most adequate for the design and the promotion of the kind of learnings that occurs in an upper level chemistry course, for example. In particular, this paper describes various pedagogical approaches implemented to promote *significant learning* in an upper level computational chemistry course.

## Computational Chemistry

In the author's institution, computational chemistry is an elective course for undergraduate chemistry seniors. Students enrolled in the MS program or the combined BS/MS program are eligible to enroll provided they meet the pre-requisites which include having completed both organic chemistry and quantum chemistry at the undergraduate level. The course has been offered in the spring quarter of every other year since 2002, although intentional design of the course based on the taxonomy of significant learning started in 2006. The average course enrollment has been twelve students ranging from eight to twenty students. Moreover, the course has consistently enrolled an almost equal number of female and male students. Most of the students have little to no research experience and no previous exposure to any kind of computational chemistry.

One goal of the course is for students to be able to determine the kind of research questions that may be effectively addressed using computational quantum chemistry as a tool. Through hands-on activities, students develop the necessary skills to apply what they learn in the course to tackle chemistry-related research questions. To accomplish these goals, students are introduced to the fundamental principles and practical applications of computational quantum chemistry.

### Course Significant Learning

One challenge in the course is to strike a balance between coverage and depth. Given the many computational chemistry approaches and methodologies, it is impractical to cover them all in just one course. Moreover, these computational approaches are not necessarily based on a single theoretical framework. Some are based on classical physics, others on quantum theory, and yet some others are based on a hybrid of these fundamental theories. The level of readiness for the students to apply and build upon these various theories constitutes another challenge. The fact that the course meets for three hours a week for 10 weeks (quarter system) needs to be factored in the design of the course. Given the aforementioned challenges, the following questions are considered: what is it that students need to learn and be able to do as a result of this course? What could realistically be achieved given the time constraints of the course, and the background knowledge of the students? How to design the course so as to help facilitate the kinds of learning students need to demonstrate in the course? How to determine that the intended learnings have occurred? As it turns out, the taxonomy of significant learning provides an important framework to help answer these questions. Accordingly, one component in the design of the computational chemistry course is the identification of the learning outcomes of the course, and their alignment with Fink's taxonomy of learning as detailed below.

Each of the learning outcomes below is to be read as "The student will be able to" with the sentence being completed in the specification of the outcome.

*Foundational knowledge*

- … define computational chemistry.
- … identify and explain the governing principles of computational quantum chemistry.
- … identify and describe key concepts, terminologies, approximations, and conventions.
- … describe similarities and differences between various computational quantum chemistry methods.

*Application*

- … solve a chemistry research question effectively and efficiently by
    - determining appropriate computational quantum chemistry methods to use.
    - using an appropriate computer program to carry out quantum chemistry calculations.
    - working effectively in a Linux and windows operating system environment.
    - managing complex projects.
- … present computational chemistry results both orally and in writing.
- … analyze and evaluate the quality of computational chemistry results, and propose alternate ways of improving the quality of results.

*Integration*

- … integrate computational chemistry with other branches of chemistry, and relevant disciplines such as biochemistry, organic chemistry, etc.

*Human dimension*

- … work independently and with others in a respectful and productive way to solve problems or address issues guided by scientific and ethical principles.

*Caring*

- … value computational chemistry as an essential ally in modern research in chemistry and in related disciplines.

*Learning how to learn*

- … build on what has been learned to determine what else is needed or wanted to learn about computational chemistry, and then developing concrete actions for achieving the desired new learning.

To help students meet the learning outcomes of the course, several instructional strategies and activities were used as outlined next.

## Essay Accounts

One pedagogical approach adopted in the course is an Essay assignment that reads: "*Your assignment is to use your current academic background to ponder a research question in chemistry that you are interested in, and then provide your approach in the form of a systematic methodology to address the question in a way that either completely answers it or at least provides you with significant insight about the subject matter."* (See Appendix for description of the assignment). Writing as a learning tool has been shown to be an effective approach to help students deepen their learning and understanding of a subject matter (Bean, 2011). In particular, essay assignments may be designed to incorporate higher levels of Bloom's taxonomy as exemplified in the literature on project-based learning (Halpern, 2014; Krauss & Boss, 2013). The assignment requires students to use their current knowledge in chemistry. It also promotes critical thinking (*Application* dimension). Consequently, students are given an opportunity to demonstrate sufficient depth in their thinking to formulate a chemistry question and then to make appropriate judgments about how to tackle it in an effective and efficient manner. The assignment promotes *Integration* as students need to formulate a question based first on their current academic background, and then refine the question and the ways to solve it by integrating some of the computational chemistry tools they learn in the course. As for *Caring*, students demonstrate that they already care about the content of the course by virtue of choosing to enroll in this elective course. Nonetheless, students are seen to develop a much deeper appreciation of what computational chemistry can do for them upon completion of the course in general and the Essay assignment in particular; the *Human* dimension is factored in as students are formulate a question they feel passionate about but still they are required to persuade others of the importance of solving the question.

Although only 10% of the overall grade, the Essay assignment has been instrumental in the realization of a *significant learning* experience for the students in the course. At first, most students feel at odds with the assignment because they are not used to formulating research questions, let alone developing a plan to tackle them. One key to the success of the assignment, however, is the explicit connection of the assignment to what students already know and to the things they care about. Through these connections, students interact with the course content in a more meaningful way, and become more motivated to learn. Through frequent meetings with individual students, I help them develop their initial take on the assignment, and after that, students take ownership of the assignment. As students learn more about computational chemistry, they move the assignment successfully forward in all cases. Regular contact with students is maintained to provide formative feedback prior to the submission of the Essay accounts. The continuous support from the university writing center is also vital to help students address writing issues.

### Mastering Fundamental Skills

Every class meeting is divided into two periods each of 90 minutes. The first period is devoted to the acquisition of foundational knowledge and to the development of deep learning through group discussions (about assigned readings or issues in assigned projects/activities). The second period is devoted to hands-on activities to master fundamental skills. Students are taken to the computer laboratory where they work in their assigned computer station. For students to be able to apply what they learn in the course, they need to master the following operational skills: work in and navigate between both Linux and windows computer environments; work with the computer software used to set up and carry out computational chemistry calculations, and the software used to help visualize, collect and analyze the results of the calculations. To facilitate learning and mastering of these skills, I developed a series of activities for students to engage in during class. There are additional activities for homework assignments. Each activity is given with specific learning outcomes, so that students know what it is that they will be able to do as a result of the activity. The first few hands-on activities focus on mastering numerous Linux commands that students need to use regularly such as remote login, create directories, create and edit files, and so on. At first, students feel visibly overwhelmed with the myriad commands they need to learn. In just a couple of weeks, however, students demonstrate a level of competence that is appropriate for them to work independently in a Linux system. Building upon the skills mastered, the pedagogical efforts are directed towards developing the skills necessary to work with the computer software used to run the calculations and visualize the results. Such skills include setting up and running calculations, troubleshooting, creating/editing input files, collecting and visualizing data, etc. Several in-class activities and related homework assignments are developed for students to master the mentioned skills to the point they can work independently. Students are also directed to video clips (on the web or that I prepared myself) that touch base on issues of practical relevance like setting up calculations and visualization and analysis of results. Half way through the quarter, students have acquired the skills necessary to begin working on the research project. One reason for the success of the hands-on activities is their practical nature and the on-the-spot feedback. The activities are designed in a scaffolding manner to build continuously on "small wins", that is, students develops confidence and a sense of accomplishment via the achievement of very specific targets or milestones. Students need immediate feedback since they would not be able to move on to the next step unless they succeed in the step they are working on at any given time. One feature of the hands-on activities is that it promotes peer-led teaching and learning. Students who grasp the skills more quickly than others tend to help their peers on site, or even after class. This social aspect adds to the *Human dimension* of learning, and helps narrow the gap in the performance among students with varying abilities.

### Evaluating Quality of Results

Upon mastering the basic operational skills, students start reading selected computational chemistry publications. We discussed the publications during lecture with regard to research questions addressed, methodology chosen, and results quality. These readings help provide a framework to discuss and examine the foundational knowledge being imparted in the course, i.e. the basic principles and practical applications of computational quantum chemistry methods. As part of the discussion, students work in small groups and are required to suggest ways in which the quality of the results could be improved. During the hands-on portion of the class, students are asked to reproduce themselves portions of one or more of the research publications discussed. Then, students are asked to examine whether the quality of the results could indeed be improved by implementing some of the suggestions made during the lecture discussions. Students find the activity of reproducing portions of a real research paper very reassuring and stimulating. It is also instrumental in helping students build capacity to undertake their own research project.

### Developing and Managing a Research Project

At week five, each student is assigned a project so they can apply what they are learning in the course and integrate what was learned in other courses. The project is designed to shed light into a research question in chemistry using known methodologies in chemistry and including some of the computational chemistry tools presented in the course. Each student is given a unique project, although most projects are designed to be complementary projects. In some instances, the project is assigned based on the research question proposed in the Essay assignment. Most often, students work on projects that I know can be completed in five weeks or less. The project resembles an authentic performance task (Hansen, 2011) as students are challenged to integrate and apply what they have learned to scenarios that mirror closely a real-life professional setting. Students are encouraged to discuss with one another about their individual projects. As a result, students are seen to develop and maintain constructive working relationships. Through peer interactions, students develop a learning community that enables them to learn from one another.

During the first three weeks of the project, students demand constant support, but for the final weeks students are largely independent and able to bring the project effectively to completion. Throughout the project, students experience changing and sometimes frustrating situations. Students are challenged to manage what is in essence a complex project. Students need to make decisions, organize information, plan and implement different tasks that need to work in concert to achieve the goal of the project. Students are challenged to exercise creative thinking as there are usually different yet valid approaches that can be used to develop the project, with some more efficient or effective than others. Students need to make practical decisions given the constraints of time and computer resources at hand. Moreover, the research project helps promote students' ability to become independent selfdirected learners as they reflect on, and adjust as needed, the approach or strategies used to tackle the project. I provide timely feedback and support (via email, face-to-face, over the phone, etc.) to help students learn to monitor progress, restructure priorities and tasks on the fly, and redefine some of the proposed tasks or even consider alternatives to ensure success in the long run (meaning completion of the project).

Lastly, successful completion of the project promotes students' communication skills because the students are required to write a report in the format of a scientific peer-reviewed journal and to give an oral PowerPoint presentation to the entire class by the end of the quarter. I help students with the preparation of the PowerPoint presentation both in person and by directing them to appropriate YouTube videos available on the web on how to present scientific information using PowerPoint. The ACS (American Chemical Society) writing style is used in the course. Given that this is an upper level chemistry course, students are usually familiar with the ACS style. By examining peer-reviewed articles published in journals sponsored by the American Chemical Society, students develop a more practical sense of the ACS writing style. Students also learn that different scientific journals have different citation styles. For example, students are asked to compare the writing styles in two different journals: The Journal of the American Chemical Society, and the Computational and Theoretical Chemistry journal. The former is an ACS journal, the latter is not. Additionally, students are required to make use of the university writing center for support in their writing of the final report. Since the writing center has tutors in all disciplines, including chemistry, it can assist students not only with specific issues of grammar but also with writing styles.

## Results

The success of the course is revealed by the extent to which students achieve the intended learning outcomes established for the course. In aggregate terms, most students have achieved a better than satisfactory level of competence (80% or better) every time the course has been offered (a total of 9 times since 2002). A typical grading scheme is given below

1. 30% Hands-on activities and Homework
2. 10% Essay
3. 10% Midterm
4. 40% Paper based on Assigned Project (Written in the format of a peer-reviewed journal).
5. 10% Oral defense of Paper on Assigned Project through a PowerPoint presentation given to the entire class.

The grading scale follows a standard grade range of A (90%-100%), B (80%-90%), C (70%-80%), D (60%-70%), and F < 60%. More evidence comes from the observation that by the end of the course students can actually do things they were not able to do prior to taking the course. That is, students are comfortable working in the computational chemistry environment, handling the pertinent software, setting up and running calculations, formulating research questions, designing and implementing research plans, collecting, analyzing and communicating information, evaluating the quality of results, and proposing creative ways to improve upon the results. Students' perceptions of learning, as revealed in the course evaluations, provide indirect evidence of the success of the course. A few representative comments (sampled from the different times the course has been offered) referring to aspects of the course students found most beneficial are given below:

"Learning how to use the computer programs to run calculations"

"The final project allowed me the opportunity to see the vast applications of computational chemistry while also learning the challenges associated with working in this field"

"The in-class work, it gave me the hands on experience that I would need instead of just having pure reading material"

"I enjoyed replicating data from a previous publication"

"Just understanding the basic tools and the information that can be gleaned using computational chemistry is useful. It will be a useful perspective to have in the following chemistry courses"

"It helped in showing how all previous courses can bring help to computational chemistry; it made the understanding of it more helpful"

One impressive outcome is the fact that some students continue working in their assigned project well after the course is over. These students want to finish their projects at a level acceptable for publication in a peer-reviewed journal. As a result, there have been eight publications resulting largely by the students' motivation, dedication and commitment to continue learning: (Parra, Knewstub, Kusion, & Moreno, 2019; Falk & Moses, 2015; Parra & Streu, 2011; Parra & Hill, 2010; Parra & Ohlssen, 2008; Parra, Arena, & Sankissa, 2007; Gharbonpour, Wemhoff, Kofoed, & Parra, 2007; Parra, Yoo, & Wemhoff, 2006). Some students have incorporated what they learned in the course to other academic aspects of their lives, such as for their Honors Program Thesis, or to continue into MS/BS option where they use computational chemistry as an ally.

## Discussion and Conclusions

Students' feedback and my own professional development have been instrumental in changes made to the course over the years. For example, in the first two offerings of the course, I placed emphasized breadth over depth. I was following the model I experienced as a student in my computational chemistry courses. Most of the textbooks I considered for the course also favors breadth over depth. Accordingly, I spent much time on the theoretical foundations of computational chemistry sacrificing valuable hands-on practice. As one student put it, the course was "interesting but overwhelming". Suggestions from students included focusing on one computational chemistry approach, and adding more depth to the assigned projects. I searched around for best teaching practices that could be adapted to improve my teaching and hence the learning experiences of my students. When I became aware of Fink’s taxonomy, I found it to be an adequate framework to plan and design the course. I started implementing the significant learning taxonomy in 2006. Since then, the course focuses on the approach to computational chemistry based on molecular orbital theory. Hands-on activities in the course has increased, and scaffolding for the assigned projects are more intentional.

One striking feature of the course that started with the 2006 offering is the peer-reviewed publications by the students based on their projects. No such publications came out from the 2002 and 2004 offerings. Overall, the taxonomy of significant learning has proven to be an important reference framework in the design, implementation, and assessment of the course since 2006. The synergistic aspect of the various learning experiences that students are exposed to in the course is noteworthy. In planning the course, I consider building upon the strengths and prior knowledge of the students. The importance of time limitations cannot be overestimated. For example, the possibility of publishing the research with students from a course like this is perhaps unrealistic. Therefore, publishing is not part of the course grading. Moreover, publication quality requires what is known as “high level” calculations. In practical terms, this translates into very time and computer-resource demanding calculations that students would not be able to meet. This is especially true because the computer resources used are for teaching rather than for research purposes.

The publications originated in this course were possible because of a combination of several factors: students’ motivation to continue working on their projects after the course ended; students using my research lab computers to carry out publication-quality calculations; students still having my support. The number of students in the course is also a consideration. The supervision and support of individual research projects become increasingly more difficult and perhaps impractical as the number of students increases. With twenty students enrolled in 2018, for example, the research projects were designed for students to work in pairs. In other disciplines, it may even be more difficult to publish within the time window of a course. For instance, a course where students engage in research that involves human subjects will need approval from the Institutional Review Board or IRB approval. The process of getting IRB approval itself takes time making publication unlikely during the course lifetime.

Some additional considerations made when planning and teaching the course include:

- Make explicit the learning outcomes for the course.
- Provide guidance for students to work with content in meaningful ways.
- Align learning outcomes and the instructional strategies selected for the course. In particular, provide students with ample opportunities to engage in learning activities that are explicitly designed to help them develop and apply key skills in relevant tasks.
- Use assessment methods that align with the course learning outcomes.

- Develop rubrics and descriptive criteria for the desired outcomes, so that students know what they need to do to demonstrate the level of achievement expected of them.
- Rely on various forms of evidence to determine the quality and extent of learning. For example, evidence includes many performance tasks that challenge students to use judgement and innovation while demonstrating their ability to use knowledge and skills attained in the course.
- Inform students of relevant learning support resources within and outside the university. For example, the university center for writing based learning, the university library, and a variety of online resources.
- Provide opportunities for frequent and varied assessment activities to facilitate timely and targeted feedback to students. Especially to help students learn how to monitor their own progress.
- Create a course climate that fosters good interactions among students and with the instructor.
- Use a scaffolding approach so that students can move gradually from a beginning to a mastery level through a continual sequence of "small" wins that encourage the heart, and of "small" failures that prompt reflection and ability to learn from mistakes.

Promoting significant learning is worthwhile, but it does require a great deal of commitment from the part of both the instructor and the students. Achieving significant learning demands purposeful planning and consideration of such things as the nature of the course (undergraduate *vs* graduate, and upper *vs* lower levels), the interconnectedness of all learning activities, the number of students, and the time available for instructor and students to engage with the course. The intentional design and assessment of activities aligned with the learning domains in Fink's taxonomy is especially tricky, but there are helpful books (Angelo & Cross, 1993; Barkley & Major, 2016). Examples of application in various disciplines exist including religious studies (Jones & Hilaire, 2012), as well as special education, Spanish, biology, economics and others (Fink & Fink, 2009; Levine-Fallahi, 2008). These examples demonstrate the diverse ways in which the taxonomy of significant learning has been used. Interestingly, examples of Fink's taxonomy in chemistry education research (Cooper & Stowe, 2018) appears to be missing illustrating the paucity of information in this area and the need for publications like the work presented here.

In contrast, examples of application in chemistry of Bloom's taxonomy (McGuire, 2015), SOLO taxonomy (Hodges & Harvey, 2003), and Marzano's taxonomy (Toledo & Dubas, 2016) can be found. The need for further research and applications of the significant learning taxonomy is apparent. Given the known high attrition rates in general chemistry (Ye, Shuniak, Oueini, Robert, & Lewis, 2016), this course is an excellent candidate to explore ways of improving students learning experiences and performance using the taxonomy of significant learning, and to compare the results with those from other learning taxonomies. I am exploring this possibility in my general chemistry course, in particular by incorporating learning activities designed to support the *Learning how to learn* dimension in synergy with the *Foundational* and *Application* dimensions. As for the computational chemistry course, I plan to strengthen the *Integration* dimension further by having students consider and tackle issues in computer-aided drug design and atmospheric chemistry. I also plan to challenge students to consider how computational chemistry could be integrated into and applied to chemical education.

## Conflicts of Interest

The author declare that there is no conflict of interest regarding the publication of this article.

## References

Ambrose, S. A., Bridges M. W., DiPietro, M., Lovett, M. C., & Norman, M. K. (2010). *How learning works: seven research-based principles for smart teaching.* San Francisco, CA: Josey-Bass.

Anderson, L., & Krathwohl, D. (Eds.). (2001). *A taxonomy for learning, teaching, and assessing: A revision of Bloom's taxonomy of educational objectives—Complete edition*. New York, NY: Addison Wesley Longman.

Angelo, T. A., & Cross, P. K. (1993). *Classroom assessment techniques: a handbook for college teachers*. San Francisco, Calif: Josey-Bass.

Barkley, E. F., & Major, C. H. (2016). *Learning assessment techniques.* San Francisco, CA: Josey-Bass.

Bean, J.C. (2011). *Engaging ideas: The professor's guide to integrating writing, critical thinking, and active learning in the classroom* ($2^{nd}$ Ed.). San Francisco, CA: Josey-Bass.

Biggs, J. B., & Collis, K. F. (1982). *Evaluating the quality of learning: the SOLO taxonomy.* New York: Academic Press.

Biggs, J. (2003). *Teaching for quality Learning at university* ($2^{nd}$ Ed.). Maidenhead, Berkshire, United Kingdom. SRHE, and Open University Press.

Bloom, B. S. (Ed.). (1956). *Taxonomy of educational objectives, Book 1: the cognitive domain.* New York: Longman.

Bransford, J., Brown, A. L., Cocking, R. R., & National Research Council (U.S.). (1999). *How people learn: Brain, mind, experience, and school.* Washington, D.C: National Academy Press.

Cooper, M. M. & Stowe, R. L. (2018). Chemistry education research: From personal empiricism to evidence, theory, and informed practice. *Chem. Rev.,* 118: 6053-6087.

Davis, J. R., & Arend, B. D. (2013). *Facilitating seven ways of learning: a resource for more purposeful, effective, and enjoyable college teaching.* Sterling, VA: Stylus.

Falk, N. & Moses, A. (2015). Diol-mediated versus water-mediated proton transfer reactions. *DePaul Discoveries,* 4(1), 1-7.

Fink, L. D. & Fink, A. K. (2009). *Designing significant learning experiences: Voices of experience*. Issue #119 in the "New Directions for Teaching and Learning" series. San Francisco: Jossey-Bass.

Fink, L. D. (2013). *Creating significant learning experiences: An integrated approach to designing college courses, revised and updated*. Hoboken, NJ: Wiley.

Ghorbanpour, M., Wemhoff, M. P., Kofoed, P. & Parra, R. D. (2007). Intramolecular hydrogen bonding effects on chelate binding of ions by aromatic amides: A DFT study. *Journal of Undergraduate Chemistry Research,* 6, 135-139.

Halpern, D. F. (2014). *Thought and knowledge: An introduction to critical thinking* (5th Ed.). New York, NY: Psychology Press.

Hansen, E. J. (2011). *Idea-based learning: A course design process to promote conceptual understanding*. Sterling, VA: Stylus.

Hodges, C. L. & Harvey C. L. (2003). Evaluation of student learning in organic chemistry using the SOLO taxonomy. *J. Chem. Ed.*, 80(7), 785-787.

Jones, J. L., Hilaire, R. S. (2012). Creating significant learning experiences: A case study in the college religion classroom. *The Journal of Effective Teaching*, 12(3), 34-43.

Knowles, M. S., Holton, E. F., Swanson, R. A. (2015). *The adult learner: The definitive classic in adult education and human resource development* (8th Ed.) New York, NY: Routledge.

Krauss, J. & Boss, S. (2013). *Thinking through project-based learning: Guiding deeper inquiry*. Corwin Press.

Lederman, N. G., & Lederman, J. S. (2015). What is a theoretical framework? A practical answer. *J Sci Teacher Educ, 26, 593-597.*

Levine, L. E., Fallahi, C. R., Nicoll-Senft, J. M., Tessier, J. T., Watson, C. L., & Wood, R. M. (2008). Creating significant learning experiences across disciplines. *College Teaching*, 56(4), 247-254.

McGuire, S. Y. (2015). *Teach students how to learn: Strategies you can incorporate into any course to improve student metacognition, study skills, and motivation*. Sterling, VA: Stylus.

Marzano, R., & Kendall, J. (2007). *The new taxonomy of educational objectives* (2nd Ed.)*. Thousand Oaks, CA: Corwin Press.*

Parra, R. D., Yoo, B. & Wemhoff, M. (2006). Conformational stability of a model macrocycle tetraamide: an ab initio study. *Journal of Physical chemistry A.,* 110, 4487-4494.

Parra, R. D., Arena, A., & Sankisa, S. (2007). Conformational preferences of carbonic acid and its sulfur derivatives, $H_2C(=X)O_{2-n}S_n$ ( X = O/S; n = 0-2). *Journal of Molecular Structure,* 815, 31-40.

Parra, R. D. & Ohlssen, J. (2008). Cooperativity in intramolecular bifurcated hydrogen bonds: An ab Initio study. *Journal of Physical chemistry A,* 112, 3492-3498.

Parra. R. D. & Hill, B. (2010). Conformational analysis of n-fluorine, 2,2'-X (n = 3 or 3'; X = bifuran, bithiophene, or thienylfuran): Ab initio, density functional, and multi-coefficient correlation results. *Journal of Molecular Structure,* 940, 61-69.

Parra, R. D. & Streu, K. (2011). Cooperative effects in regular and bifurcated intramolecular OH…O=C interactions: A computational study. *Computational and Theoretical Chemistry,* 977, 181-187.

Parra, R. D., Knewstub, S., Kusion, P., & Moreno, G. (2019).Cyclic dimers of formamidine with its N halogenated formamidine analogues: Structure, energetics, and proton-halonium transfer. *Computational and Theoretical Chemistry,* 1153, 1-11.

Toledo, S. & Dubas, J. (2016). Encouraging higher-order thinking in general chemistry by scaffolding student learning using Marzano's taxonomy. *J. Chem. Ed.*, 93, 64-69.

Ye, L., Shuniak, C., Oueini R., Robert, J. & Lewis, S. (2016). Can they succeed? Exploring at-risk students' study habits in college general chemistry. *Chem. Educ. Res. Pract.*, 17, 878-892.

## Appendix

### ESSAY

This assignment represents 10% of your overall grade. You will complete this assignment in two different accounts called Account 1 and Account 2 respectively. Each one of these Accounts deals with essentially the same assignment. However, the accounts are expected to be written at increasingly deeper levels of critical thinking. Accordingly, the 10% is distributed to mirror the increased expectations as follows: Account 1 (3%) and Account 2 (7%).

PURPOSE:
The main purpose of this activity is to provide you with an opportunity to demonstrate your ability to make appropriate judgments about how to tackle a research question in chemistry in an effective and efficient manner. Thus, what matters the most here is the quality of your critical thinking represented in this essay.

ASSIGNMENT:

Your assignment is to use your current academic background to ponder a research question in chemistry that you are interested in, and then provide your approach in the form of a systematic methodology to address the question in a way that either completely answers it or at least provides you with significant insight about the subject matter.

FORMAT: Your essay will not be composed of separate sections, but it should include the following components:

- **Claim:** There should be a clearly identifiable research question in your first paragraph. The research question should be suitable for investigation using the tools provided by the field of chemistry, especially including computational chemistry. *Please note that the research question that you formulate in Essay Account 1 most likely will change or be refined as you developed a better understanding of what computational chemistry can do to assist you in your research. The expected gradual change in your formulation of the research question and the way you will tackle it should appear in your Essay Account 2.*
- **Analysis**: Identify and describe the research strategy you have deemed appropriate to tackle your research question. It is critical that you are not simply creating a bulleted list of steps to follow in your quest to answer your research question. Rather, you should be writing fully developed paragraphs to support your chosen methodology.
- **Persuasive Elements**: Think about what would persuade your specific audience and use that to make your points more effective. It will be important to provide the reason or motivation that you have in pursuing this research.

AUDIENCE: Imagine that you are writing to a group of people who may be willing to finance your research so long as you convince them that the question you are addressing is an important one, that it can be addressed satisfactorily with the methodology you propose, and that you understand the requirements for solving the problem.

REQUIREMENTS: 4-5 pages, double spaced, 12 pt. Times New Roman font, 1-inch margins

DUE DATES:
Account 1: Thursday, April 14th 2016
Account 2: Thursday, May 25th 2016