Physical Chemistry: A Curriculum for 2004 and Beyond

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Abstract: Physical chemistry education combines the content of physical chemistry with pedagogical insights on teaching. Creative tension results from intertwining the abstract nature of the content with how to teach and assess the content within the time constraints of a curriculum. In this paper we address what physical chemistry content needs to be included in lecture and laboratory, what education research suggests about how students learn, and what presentation methods appear to help increase student knowledge. The incorporation of technological tools into the curriculum is discussed as a means to increase student conceptual understanding. We envision a changed physical chemistry class structure focused on the student with the instructor using a wide range of instructional tools including traditional lecture, cooperative assignments, computer software, modern concept-based laboratories, and an assessment scheme based on student learning.

1. Introduction

Any discussion about teaching physical chemistry in the 21st century requires a definition of physical chemistry. We will use the one developed by the Société Francaise de Chimie - Division de Chimie Physique. The Société wrote [1],

> Physical chemistry aims at understanding the structure, properties and transformations of matter, from bulk behavior down to mechanisms at the molecular level. It is the role of the physical chemist to collect, collate and analyze experimental data from all branches of chemistry and to construct predictive models. As such, physical chemistry underlies much of modern science and is a motor driving advances in a very wide range of fields. Building on information and concepts from chemistry, physics and mathematics, physical chemistry contributes to and is stimulated by areas as diverse as medicine, molecular biology, biochemistry, molecular engineering, chemical engineering, materials science and earth sciences.

More broadly stated, physical chemistry is what physical chemists do. Physical chemistry has seen dramatic changes in the discipline's scope with a commensurate increase in the number and type of research areas. The physical chemistry curriculum has also seen significant changes from the material in Glasstone [2], much of which appears in modern general chemistry, to the breadth of material available in 2004 [3–5]. The physical chemist's classroom tools have also changed from slide rules, log tables, and chalkboards to graphing calculators, computers with symbolic algebra and computational chemistry software, Internet resources, and smart boards. One must also consider changes in student attitudes and our understanding of how students learn.

In spite of increased textbook content, the time allocated to physical chemistry in the typical bachelor's level chemistry program has continued to prevent examination of all recommended topics. Additionally there are questions of how thoroughly any topic can be covered in the 90 classroom hours of a one-year course, how the students' level of preparation for the course controls the content and depth of study, and how chemical concepts and pedagogy work together to create a modern image of physical chemistry while addressing fundamental topics. Further consideration must also be given to the various programs requiring courses in physical chemistry. These span fields ranging from biology, chemical engineering, and forensic science, to law. There is considerable difference between a course for the small fraction of students taking physical chemistry to become physical chemists, a course providing an overview of what physical chemists do, and a course offering students an opportunity to use the tools of modern physical chemistry. Finally, because physical chemistry bridges courses in physics, chemistry, and mathematics, it is the course in which students can develop the complex critical thinking skills required by scientists working on projects with interdisciplinary foci.

2. Background

Physical chemistry education has changed significantly over the last 100+ years, just as the discipline itself has changed [6]. Originally founded as a discipline focused on thermodynamics and electrochemistry, the field now encompasses subareas too numerous to list and contributes to the study of almost all the other subdisciplines of chemistry, interdisciplinary areas within chemistry, and many multidisciplinary areas of which chemistry is a part.

Although physical chemistry education has been discussed since the beginning of the discipline [6–8], in this review we will focus on publications since 1980. We begin with the results of a 1984 ACS invitational workshop [9] where a group of chemists and chemical engineers discussed the state of physical chemistry education, made several recommendations about where particular concepts fit within physical chemistry, and suggested the removal of several topics from the curriculum. These recommendations included the movement of electrochemistry to the analytical chemistry courses, the incorporation of lasers and computers into the curriculum, and

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the use of more relevant examples from chemical engineering. An outcome of the workshop was a sourcebook of reference material for physical chemistry teachers [10] describing the views of several chemists and chemical engineers on physical chemistry topics, particularly with regard to the interface between chemistry and chemical engineering.

In 1992 "The Problem with P. Chem" [11] again confronted the issue of what to include in the physical chemistry curriculum. These authors wrote that it was extremely important to make the physical chemistry curriculum reflect what physical chemists do, and that the lecture and laboratory curriculum required updating by replacing many antiquated exercises with modern experiments using modern techniques and instruments. In addition, the authors recommended that lecture shift away from the classical fields to make room for relevant/current scientific examples and to increase the emphasis on kinetics and quantum mechanics. Emphasized material should also fully incorporate the use of molecular modeling, simulation, and visualization software into the curriculum. A monograph containing materials from NSF and Pew Foundation funded projects [12] gave useful teaching points for the lecture and detailed experimental specifics for a number of laboratory exercises. These experiments are still relevant and can be readily adopted by instructors developing updated physical chemistry laboratory curricula.

In 2003 the Committee on Professional Training (CPT) of the American Chemical Society published a revised set of guidelines for the undergraduate physical chemistry experience [13]. These guidelines call for a focused experience at the conclusion of which students will understand the fundamental concepts in physical chemistry. They should also have a firm grasp of how the various parts of physical chemistry relate to each other, to the other subdisciplines of chemistry, and to the various fields for which physical chemistry provides fundamental support.

As part of the New Traditions curriculum systemic reform project, a group of physical chemists met to discuss the state and future of physical chemistry education [14]. They concluded that problems existed within the curriculum, especially with regard to overuse of mathematical manipulation and a corresponding under-emphasis of conceptual development. In addition, the mode of instruction used in the course needed to become more student-centered through the use of guided inquiry and cooperative learning strategies.

Even as the curriculum has been modernized, new developments in learning theories, classroom technology, and the science itself have caused renewed calls for including additional topics in the curriculum. These include polymer chemistry [15, 16], materials science [17–19], and nanomaterials, all subjects that require thorough understanding of physical chemistry.

3. Modern Physical Chemistry

Recent advances in the work performed by physical chemists have resulted in calls for the inclusion of even more materials from modern research methods into the physical chemistry lecture and laboratory curriculum. Without attempting to enumerate all of these projects, it is worthwhile to discuss a few of the advances likely to affect the curriculum.

Theoretical advances and advances in hardware and software have changed the nature of chemistry through the development of new models and through the application of existing models to more complex systems. The development of density functional techniques [20] for structural energy calculations has had a tremendous influence on how calculations are performed. In these computational methods, the molecular orbital picture is abandoned in favor of directly determining the electron density within the molecule. The set of equations describing the electron density is solved directly rather than by taking the complex conjugate of the wavefunction. When information is not needed on the particular orbital energies, these calculations have proved to be more efficient than traditional ab initio methods while still providing results suitable for comparison with experiment. Another major advance, improvements in computational methods and computer power, has reduced the time and effort required; fewer approximations need to be made to perform a calculation on any given molecule [20]. Now, physical chemists can routinely use the tools of quantum mechanics to examine moderately sized molecules and the methods of classical mechanics to study conformation equilibria in biomolecules [21]. In addition, the quantum dynamics of reactive systems are under examination from both theoreticians and experimentalists at an ever-increasing level of detail, even to the level of dynamic resonances for particular quantum states at particular energies [22].

As the discipline becomes more interested in large molecules and larger ensembles of molecules, a theoretical means of understanding the system needs to be developed. Classical mechanics provides such a tool through the development of force fields between atoms within a molecule and between molecules. Molecular mechanics and molecular dynamics algorithms are used to model the motions of molecules about their equilibrium structure. This motion can be used to understand topics as varied as protein conformational equilibrium [23, 24] and light scattering by small molecules in solution [25].

The study of molecular collision dynamics has advanced markedly with the development of faster, time-based probes of atomic motion from the picosecond to the femtosecond time scales. On the femtosecond time scale, the details of atomic motion become observable in the course of a collision [26], as do the effects of quantum interferences within a state [22]. A second major experimental influence is the ability to image, detect, and perform reactions on different surface morphologies using the various surface-active methods for reactions and analysis. The development of surface morphological experiments can provide insights into the action of catalytic surfaces and the importance of dislocations on the surfaces [27].

As the field of physical chemistry has broadened, the domains in which physical chemistry have an impact now range from the discovery and characterization of fullerenes [28] and Bose–Einstein condensates [29] to the modeling of complex atmospheric systems [30] and reactive system design [30, 31]. Even the well-characterized field of thermodynamics is experiencing a renaissance through its application to materials on the micro- and macroscopic levels [32].

4. Instructional Issues

a. Core Concepts and Critical Thinking in Modern Physical Chemistry. What are the goals for a physical chemistry course? First, physical chemists must transmit the discipline's critical ideas while keeping in mind that all content cannot be included in a one-year course. Second, instructors must develop in students the fundamental skills for using mathematical models and an understanding of their significance and limitations. Third, physical chemistry teachers are charged with further developing in students those critical thinking skills that relate to understanding how chemistry works.

Core curriculum key areas include thermodynamics, chemical dynamics, quantum chemistry, and basic equilibrium statistical mechanics. These are traditionally split into semesters where thermodynamics or quantum chemistry dominates and statistical thermodynamics or dynamics squeeze into a few weeks. Thermodynamics incorporates the traditional suite of state functions, ideal and real gases, and chemical and phase equilibria. Quantum chemistry topics include some historical background, the Schrödinger equation, model systems, the hydrogen and multielectron atoms, modern molecular orbital theory, and spectroscopy. Chemical dynamics typically contains kinetic molecular theory, transport properties, simple-order reactions, transition-state theory, and activated-complex theory, while statistical thermodynamics consists of development of the partition function as a product of electronic, translational, rotational, and vibrational contributions. In addition some would argue for the inclusion of polymer chemistry, especially with respect to biomacromolecules, solid-state chemistry, crystallography [33, 34], group theory, or even an introduction to molecular mechanics and molecular dynamics [35, 36]. How interesting it would be to study dynamics using molecular dynamics, a state-of-the-art application of classic concepts, as the focus for a very modern course.

In physical chemistry, instructors are also asked to provide a basic review of mathematics and to take responsibility for satisfying the writing requirement for chemistry graduates through laboratory writing intensive course designations. It is clear that an instructor would have to talk very fast, use the best electronic presentation tools, and provide copious handouts to students to meet all possible course expectations. The consequences of such actions are rarely positive, namely, alienated students and frustrated faculty, low exam scores, and poor concept retention. These consequences motivate the search for different and more effective methods of instruction.

One factor affecting how we teach is the extent to which students understand what we teach, that is, that physical chemistry concepts are ingrained into student's brains and connected to previously acquired knowledge. To demonstrate that the concepts are ingrained and connected, students must show that they understand the meaning of textual material, mathematical equations, and word problems found in lecture and laboratory applications. Demonstration of the ability to understand various modes of concept presentation and assessment is further evidence for the logical/abstract reasoning ability necessary for success in physical chemistry.

Thus, another goal of a physical chemistry course is to help students develop logical thinking patterns while promoting their ability to process more abstract information. This goal extends past the complex correct thinking upon which traditional problem solving instruction focuses [37–39]. Creating complex correct thinking in lecture, where the focus is the presentation of concepts and algorithms for solving standard problems, is easy. Logical thinking requires the ability to follow the path from principles to conclusions. Critical thinking extends this by requiring judgment on a proof's validity and an analysis of any limitations on a conclusion or model [40]. In physical chemistry, logical thinking is used to create models in mathematical form while critical thinking allows exploration of the model's range of applicability while striving for its most elegant representation. It is not enough to tell students about validity and limits, they must practice using their own thinking processes to internalize and use the skill effectively.

We have come full circle. The core concepts must be taught in such a way that students develop the requisite thinking skills. Selected topics must permit deeper understanding of both content and intellectual processes. Derivations should be few and reserved only for the most important concepts. For example, one should not take class time to derive the Poiseuille equation for laminar flow or the freezing point depression equation.

b. Time Constraints and Selectivity in the Curriculum. A burning issue for physical chemistry teachers is what to present and the depth of exposition in the one-year course. All of the concepts contained in physical chemistry texts cannot be presented to students within the time allowed. Time constraints become even more important in guided-inquiry or cooperative-learning class formats. The key is appropriate topic choice.

The range of activities pursued by modern chemists and the role of physical chemistry in the work of all chemists provides some guidance for making choices in the curriculum. In any group of 100 chemistry majors only a small fraction will pursue physical chemistry as a career. Others will become organic chemists, biochemists, analytical chemists, physicians or dentists, etc. The students and their potential interests determine what material is chosen. Topics included in the curriculum should be those essential for success as a thinking scientist. A course focused on the basic concepts of thermodynamics and equilibrium with an extensive study of kinetic theory and chemical kinetics and a strong emphasis on quantum chemistry applied to spectroscopy would be excellent. There is no need for detailed study of multiple particle-in-a-box problems. Although a clear outline of the hydrogen atom solution is essential, the full details can be relegated to an appendix in undergraduate courses. More important is the development of an understanding of the electron probability distribution function that leads to bonding concepts. A student finishing one year of physical chemistry should have enough quantum chemistry to understand the basic concepts used in molecular modeling and computational chemistry. Students should know why a basis set exists and some computational methods and their limitations [41]. They should know what a force field is and be able to use the harmonic oscillator model for bond stretching and bending. They should understand the nature of a potential energy surface as used in organic chemistry and be able to locate transition states and interpret potential energy surfaces with saddle points. In addition to the previously mentioned concepts, a strong emphasis on spectroscopy and its use in solving chemical problems is essential for all chemists.

In engineering environments there should be a greater emphasis on standard chemical thermodynamics and traditional phase equilibrium topics. A heavy dose of chemical kinetics including the use of stochastic modeling of reactive systems would be very appropriate [42]. Engineering students should also be given a firm foundation in modern computational techniques with an emphasis on the use of symbolic algebra and the exploration of mathematical models. Quantum chemistry should focus on the underlying mathematical models for each spectroscopic technique. Chemistry majors would be well trained in this broadly sketched curriculum.

In a course with a predominance of biochemistry majors there needs to be greater emphasis on thermodynamics and the application of spectroscopy to biochemical problems. Students must be fluent with use of the physiological standard state. The phase rule and electrochemistry become less important except as applied to determining equilibrium constants. Polymer and macromolecule topics should dominate in examples used. A greater emphasis on molecular motion, membrane transport, and colligative properties along with modern techniques for determining the molecular weight of macromolecules is essential. Given the importance of crystallography [34] and mass spectrometry [43] to the study of biomacromolecules, a solid introduction to these techniques must not be overlooked in a physical chemistry curriculum for biochemistry majors. Several texts contain an assortment of topics for the undergraduate physical chemistry or biophysical chemistry course [44, 45].

c. Mathematics and Physics Background of Students. The mathematical preparation of physical chemistry students has long been a concern [7, 46–48]. In 2000 a group of chemists discussed the relationship between the mathematics and chemistry curricula. Among the invited chemistry participants were physical chemists using mathematics extensively in their courses and research. Clearly, a solid foundation in mathematics is required for all chemistry students. Their recommendation [49], like that of the ACS CPT, was that all chemistry majors should have calculus through multivariable calculus. For potential Ph.D. students, additional courses in mathematics, including linear algebra and/or differential equations, are highly recommended.

During the 2000 meeting, suggestions were made for sharing the task of enriching the mathematical preparation of chemistry students. Responsibility for integral and differential calculus; creating, using and interpreting graphs; making estimates and creating assumptions; using iterative techniques; handling different coordinate systems; applying numerical methods; using number systems; and handling 3-D geometry lie fully with mathematicians teaching calculus and other courses. Students must enter physical chemistry courses with flexible skills and the ability to add to those skills on a need-to-know basis. Few students will come to physical chemistry with their mathematical skills in a finely honed condition because their mathematics instruction and physical chemistry may be separated by a period of time.

Physical chemists should not treat the physical chemistry course as a mathematics course. We do have some responsibility for introducing additional mathematical concepts to our students, but not for training mathematicians. First we need to remind students of the essential calculus skills that all undergraduate physical chemists need. Exact and inexact differentials and partial differentials can be introduced during the development of course topics. Graphing techniques should be emphasized throughout. Students are better served by being able to interpret and use graphs than by derivations of laws learned in general chemistry. There is no reason for present-day students to perform hand calculations, such as applying Simpson's rule. Quick estimates of areas or software generated quantitative evaluations should be routinely employed [49]. Students must be familiar with statistics (beyond the level found in quantitative analysis courses) that includes randomness, probability, distributions, Monte Carlo methods as applied in chemistry [50], and multidimensional Gaussian and Maxwell–Boltzmann distributions. Students must develop the ability to visualize systems on a molecular scale and to apply models representing molecular-scale processes. Other topics to introduce to students in a physical chemistry context are the use of operators, matrix methods, basis functions, orthonormal functions, function symmetry, and linear and nonlinear curve fitting.

d. Nature of Calculus Reform. That physical chemistry instruction relies upon the student's understanding of physics and mathematics is beyond question. Traditionally taught courses rely heavily on students' abilities to perform algebraic manipulations; to analytically evaluate both derivatives and integrals in multiple dimensions; and to solve some simple problems in differential equations, linear algebra, and complex variables. Typically, the mathematics needed for the last few topics is taught in the context of the physical chemistry in which it is used.

During the 1980s mathematics instruction was strongly influenced by the NSF-funded calculus reform projects, a reform that now also pervades mathematics education for the years preceding and following calculus instruction [51]. Students in the "new calculus" typically spend less time solving problems analytically, focusing instead on the meaning of the derivative as the slope of the curve and the integral as the area underneath the curve. Also, students experiencing this new curriculum will have a greater facility with symbolic algebra software, such as Mathematica, Maple, or Mathcad, or graphing calculators because these are commonly an integral part of instruction. Certain skills, especially algebraic manipulation skills, have been de-emphasized. It is an open question as to whether the new mode of calculus instruction enhances students' abilities in a traditionally taught physical chemistry course. In courses emphasizing numerical methods for the solution of problems, it is expected that the new mode of calculus instruction would improve students' abilities to perform the tasks expected of them. On the other hand, the lower emphasis on algebraic manipulation may make it more difficult for students to follow the logical presentation of mathematical models in standard physical chemistry texts.

5. Laboratory

a. Dichotomy between Precision of Measurement and Understanding Concepts. In the past, a reason for using mathematics in physical chemistry was the emphasis on data reduction, rigorous error propagation, and statistical analysis required for the training of chemists. Students spent many hours doing calculations that are now routinely performed using appropriate software. It is not clear that these laboratory exercises led to a greater understanding of error analysis or the concepts underlying the data collected. An artifact of this approach was an emphasis on precision of data acquisition especially in solution preparation and use of volumetric glassware. As examples we note a methyl acetate hydrolysis experiment with its numerous titrations, and experiments focusing on the use of viscometers, pycnomometers, and tensiometers. Given the rich range of industrial and academic specialties of physical chemists, it is questionable if experiments focused on physical property measurement and subsequent error analyses add much to the laboratory curriculum. The details of error analysis are best left to the physics and analytical chemistry laboratory courses and then carried over to the physical chemistry course. The physical chemistry laboratory should be a place where chemical concepts based on data obtained through careful experimentation are fully examined. The results obtained including error analysis are meaningless if students do not understand the chemical concepts.

Given that the physical chemistry laboratory should be concept driven, we then ask what concepts should be included and how they should be developed. Most departments must maximize use of limited resources. Thus, a modern concept-driven laboratory curriculum can be formed around a few well-chosen instruments including UV–vis spectrometers, FTIR spectrometers, calorimeters, computers, computational chemistry software, and some laser equipment. Other spectrometers, such as a polarimeter and a fluorescence spectrometer, would be useful. Faculty can use other departmental instruments, for example, FTNMR, and GC–Mass spectrometers. Departments with limited resources can enter consortia in order to access a high-field NMR [52]. The prices of small solid-state lasers and circular dichroism and Raman spectrometers make entry-level devices suitable for a concept-driven undergraduate instruction available to all departments [12, 53, 54].

b. Traditional Physical Chemistry Experiments. There is no need to discard traditional experiments. Some are excellent choices for introducing important concepts while preserving faculty sanity in the face of an evolving curriculum. Examples include analysis of the HCl/DCl IR spectrum, NMR determination of keto–enol tautomer equilibrium, and the conjugated dyes UV–vis experiment. The data analysis for many other standard experiments can be reworked to include greater computerization. For example, sucrose inversion kinetics can be updated by incorporating nonlinear curve fitting into the data analysis and eliminating the measurement of the infinite-time optical rotation. Templates for nonlinear curve fitting are easily developed using symbolic algebra software. Another example of an older experiment that can be upgraded is the viscometric determination of the molecular weight of a polymer, polystyrene, or protein, bovine serum albumin, in solution. This type of experiment is especially suited to the laboratory forming part of a biochemistry program. Examples of potentially suitable polymer experiments can be found in the literature [55]. Other classics include using polarimetry to determine a protein helix-coil transition temperature [56] or titrimetry and UV–vis spectroscopy to determine the equilibrium constants of cysteine [57]. Finally, the curriculum can be enhanced by the use of simulation software to teach complex concepts in dynamics and modeling [42, 58–60].

c. Modern Techniques. Chemistry majors find employment in a variety of fields and need to draw on skills developed during their undergraduate and graduate education. Learning modern physical chemistry techniques is essential for all students. Students should experience concept-building activities that include the use of lasers, kinetics methodologies, and computational chemistry software. Even those not planning to be physical chemists will need some experience with modeling software and the limitations of computational methods before using these tools on research projects.

The laboratory is an ideal place to introduce molecular modeling into the undergraduate physical chemistry curriculum. Molecular mechanics models apply the essential concepts of physics and calculus to a chemical problem. Relative molecular energies allow the estimation of ΔG, equilibrium constants, and reaction coordinates. For example, when students study hydrogen bonding using modeling software with appropriate visualization tools, they can focus on the structure and properties of important molecules and macromolecules. Such approaches are important as greater numbers of chemists are trained to work at the interface of biology and chemistry. Students should learn the basic terms used in modern computational chemistry in their physical chemistry course. A modern chemist reading the literature must know what a Gaussian function is, or how they are used as STO-*n*G functions, etc. to create molecular orbitals [61–66].

Linking computational chemistry to spectroscopy is the natural focus of a modern undergraduate physical chemistry laboratory. The UV–vis conjugated dyes experiment with quantum mechanical particle-in-a-box energy level calculations and enhanced with dye family structure modeling using estimated bond and box lengths leads students to a better understanding of HOMO–LUMO concepts and their relationship to UV–vis spectroscopy. In other experiments, students could compute the vibrational frequencies for set of molecules, examine normal modes of vibration, and explore the transition state in a reaction coordinate study.

The traditional FTIR rotation/vibration spectrum for HCl is easily extended to include a computational component. By demonstrating the effect of each improvement of the mathematical model of the spectrum using Mathcad, students gain greater insights into the effects of the Boltzmann distribution, degeneracy, and the partition function on spectral characteristics. Further studies may include the centrifugal stretching contribution. Even an extended exploration of the Morse potential would increase the conceptual significance of the experiment at little cost beyond that of obtaining the software and easily adapted templates. The advantage is that at each step students actively engage in the discovery of the significance of each model component and significantly increase their understanding of IR spectroscopy.

More recently, extensions of computer simulations permit students to explore and gain understanding of time-dependent spectroscopies by using a Mathcad template to model femtochemistry laser spectroscopy [67]. Important here, and attractive to students, is an animation of the time evolution of the populated states for laser-pulse excitation of an I_2 molecule. This exercise is a natural accompaniment to the wavelength-based study of the hot bands of I_2 including Franck–Condon factors [68–71].

Spectroscopy and thermodynamics can be simultaneously explored by physical chemistry experiments. The equilibria of inclusion complexes between fluorescent dyes and β-cyclodextrin can be studied as a function of temperature by monitoring spectral shifts [72–74]. Such an experiment can be implemented using a CD fluorescence spectrometer [74]. An alternative to the cyclodextrin experiment for determining equilibrium constants as a function of temperature is the traditional keto–enol tautomer experiment using a high field FTNMR [52].

Finally, laser spectroscopy should be part of the physical chemistry undergraduate laboratory. Such experiments can be found in the literature [12]. An inexpensive laser system can also provide students with an introduction to Raman spectroscopy [53, 54].

d. Why Do We Teach Laboratory Courses and What Should Students Learn in the Laboratory? Laboratory courses serve multiple purposes in the physical chemistry curriculum. The first is to teach basic manipulative skills. Skills, including the proper techniques for making solutions, weighing, and statistical data analysis, are prerequisites for success in physical chemistry. Experience with computer-interfaced instruments is developed in both the physical chemistry and instrumental analysis courses. A second purpose is to expose students to advanced spectroscopic techniques and the precise measurement of physical properties. In the physical chemistry laboratory students routinely use instruments including FTIR and UV–vis spectrometers in applications beyond obtaining a spectrum, identifying a compound, or obtaining its concentration. The focus in physical chemistry shifts to fundamental understanding of the models underlying various spectroscopic methods. The third purpose of the laboratory is to provide students with the opportunity to perform more elaborate experiments requiring higher levels of logical thinking and an integration of multiple concepts. The focus is no longer the interpretation of what and why particular results are obtained by instrumental methods. In physical chemistry, experiments are placed in a broader context. Several chemical concepts can be combined into one experiment. Detailed laboratory reports modeled after journal articles are common [75]. Examples of laboratory activities with broader contexts follow below.

In the study of dye complexation by β-cyclodextrin, students distinguish between absorption and fluorescence spectroscopy, verify that Beer's law is obeyed for fluorescence spectroscopy, and determine the equilibrium constant for the complexation reaction. At this point, spectroscopy and thermodynamics merge with standard analytical techniques, including nonlinear curve fitting. An extension has students study the equilibrium as a function of temperature to add additional thermodynamics concepts. Interpretation of the sign of ΔH and ΔS gives students insight into the different properties of dyes interacting with the same host molecule [72–74].

Another example is an examination of interstellar carbon clusters using ab initio molecular orbital calculations [76]. Students study C_3, C_4, and C_5 clusters by constructing isomers, predicting heats of formation using MO calculations, determining the most likely candidates for matching observed spectra with calculation based on stability, optimizing the geometry of the selected isomers, and predicting vibrational frequencies. Activities of this type combine many elements of modern physical chemistry. Students use and consider the appropriateness of various levels of molecular orbital calculations. They determine energy minima and saddle points based on the computed vibrational frequencies. At the end of the project, students choose a particular C_5 isomer as the one astronomers observed.

Atmospheric chemistry can be integrated into the physical chemistry curriculum using guided inquiry with a mathematical modeling template. Harvey and Sweeney apply this approach to the Chapman Cycle for the decomposition of ozone [77, 78]. First, students use the simultaneous equation solver in Mathcad to explore the effects of temperature, total pressure, initial concentrations, and rate constants on the cycle. This is followed by an advanced component that extends the study to include the effects of NO_x, HO_x, and ClO_x in the ozone reaction cycles. Throughout, Mathcad templates help students focus on the chemical concepts and gain insights into the complex mathematical representations of interesting chemical systems without the struggle of developing the complex system of differential equations, this being more of a mathematical exercise than a development of chemical understanding. Another advanced component leads students to examine the chemistry of Cl_2O_4 in the stratospheric degradation of ozone. In this project students use group theory, spectra from the literature, RHF calculations with different basis sets, and MP2/6-31G(d) level calculations to determine the most likely structure of Cl_2O_4 and to predict the spontaneity of a possible ozone-destroying reaction [79].

e. Inquiry, Discovery, Verification. An important feature of a modern physical chemistry laboratory evolves from the examples given in the previous section. Each example is based on guided inquiry and discovery of chemically interesting concepts. None of these experiments is a verification of existing data found in the typical density, viscosity, and surface tension experiments of old. Each experiment involves the use of spectroscopy and modern computational tools including ab initio calculations and/or mathematical modeling leading to a deeper understanding of the chemical model employed.

f. Costs of Implementing a Curriculum. Surprisingly the cost of implementing a modernized physical chemistry curriculum is lower than one might think. Most departments have some of the requisite instrumentation. Access to computers is rarely an issue. The cost per computer is less than \$1000 including ample-sized monitors, operating system, and software such as the MSOffice suite. A modern curriculum would also require computational chemistry software such as Spartan [80], Gaussian [81], CAChe [66], or Hyperchem [63], adding from \$500 to \$1000 per computer. Mathcad [82], Maple [83], or Mathematica [84] add another \$500 to \$1000 per computer. Other software for teaching the basic concepts of molecular modeling and computation are available on the Internet. Also, because many schools already have networked versions of software being used by engineering or mathematics departments, many students are already familiar with these tools. Physical chemistry courses can piggyback on these facilities. When symbolic algebra software is depreciated over its useful lifetime and number of students, the final departmental cost per student is comparable to that spent on disposables or chemicals. The outcome, however, is priceless.

6. Pedagogy

There are several relevant pedagogical issues to discuss, namely, models of student learning, methods of instruction, the use of goals and objectives, and assessment.

a. The Constructivist Model. The constructivist model is an extension of the work of Piaget that can be summarized in this statement: knowledge is constructed in the mind of the learner [85, 86]. This statement implies that learning requires an active state of mind. The model is confirmed by experience—active students learn more than passive students. It also explains why students harbor alternative conceptions that are resistant to instruction, especially through lecture. The literature also tells us that if learners do not tie new concepts to their pre-existing knowledge structures these concepts are discarded [40, 87].

The findings of education specialists such as Piaget [88], Bloom [89], Perry [90], King and Kitchener [91], Paul [92], Shulman [93], and Herron [94] ought to be brought into classroom practice. The significance of the “hands on/minds on” methods of instruction stem from the research done in physics instruction by Hestines [95, 96] whose research using the Force Concept Inventory showed that students did not learn concepts or change from Aristotelian to Newtonian physics frameworks of thinking by passively listening to lectures. Students had to be actively engaged in constructing these concepts and fusing them to their intellectual frameworks.

In order for learning to occur, the learner must organize their experience in terms of their own conceptual framework; learning becomes a fitting of new data into old frameworks. Those experiences not fitting existing frameworks cause adjustments to be made. Knowledge (concepts, ideas, theories, and models) becomes rebuilt and subject to further testing. This is especially important for physical chemistry students who are constantly having their preconceptions from earlier chemistry courses challenged while being asked to construct logico-mathematical models of nature. This type of knowledge construction cannot be transferred intact from the mind of the teacher to the mind of the student [97]. In fact, the teacher must metamorphose into a facilitator of learning, one who creates the environment in which framework adjustment can take place.

b. The Perry Model. Several models of student intellectual development can be used when discussing teaching and student learning. Perhaps the most useful is that proposed by Perry [90] based on studies of male Harvard students. An analogous study of women was done by Belenky et al. [98]. These ideas were later extended to chemistry [99, 100].

According to the Perry model (as adapted by Belenky et al.), students move along a series of nine stages during their academic careers. The first five stages refer to development within a discipline while the four latter stages refer to ethical and identity development. The four stages of importance for the development of young men (women) chemists are: dualism (received knowledge), multiplicity (subjective knowledge), relativism (procedural knowledge), and commitment (constructed knowledge). The dualist considers faculty and texts as the ultimate source of correct information and that there is only one truth. In the multiplist stage truth is more arbitrary and various truths are equally valid. In the relativist stage students are adept at processing and following procedures and applying “rules of adequacy” to information, judgments, and perspectives. Finally, those at the commitment stage are actively engaged in constructing knowledge and adding this knowledge to their conceptual frameworks.

Science students score at the dualist level [101] and, at best, most chemistry students are at the relativist (procedural knowledge) stage after four years of college. This means that the majority of students taking physical chemistry are still at the dualist or possibly the multiplist level. It is therefore not surprising that so many students remain algorithmic problem solvers during their entire undergraduate science careers.

An important goal for instruction is developing a student’s ability to ask substantive questions. This leads them away from solving artificial algorithmic type problems [37, 38] toward solving complex real problems [102]. Essentially, students must be able to figure things out, to reason things through. This requires a shift in focus away from content and toward intellectual abilities through the application of the elements of reasoning, an understanding of the traits of the reasoning mind, and maintenance of standards for reasoning [92]. This is why physical chemistry is so hard for so many students. We are asking students to do what they are not prepared to do. We must refocus the curriculum to solve this problem so that the requisite reasoning skills are developed along with the construction of physical chemistry concepts.

c. Methods of Instruction. Teaching is often thought of as synonymous with lecturing, implying that to teach well one must present clear and interesting lectures, including a bit of class participation with good use of instructional tools such as electronic and chalkboard presentations, etc. Nevertheless, as Angelo and Cross [103] point out: "learning can and often does take place without the benefit of teaching— and sometimes even in spite of it—but there is no such thing as effective teaching in the absence of learning." A corollary might be that a lack of student success can result in frustration and disenchantment on both sides of the podium. Newer modes of instruction offer the possibility of enhancing the classroom learning experience. These methods go by various names including active learning [104], cooperative learning [105], guided inquiry [106, 107], structured guided reading (T.J. Zielinski, unpublished), process learning [108], cooperative learning laboratory projects [109, 110], and discovery laboratories [111].

Furthermore, the logical order that a physical chemistry lecture follows is not always the best order for the learner. This order, evolving out of the careful restructuring of concepts made by instructors and textbook authors, does not match the novice’s ability to process information and construct connections within their existing frameworks. In fact, the carefully prepared lecture is more likely to reinforce dualist thinking while providing a form of entertainment. It is only when students are alone struggling over homework that they realize that they do not understand how to do physical chemistry. Problems with long sets of data or several conceptual parts are especially frustrating for students. Lectures play to the student comfort zone. Learning requires a degree of intellectual discomfort. Currently held concepts must be challenged to make way for the beginnings of dialogues that lead to deeper understanding. Concept disequilibrium permits students to be more willing to consider new ideas and explanations.

d. Goals and Objectives. Effective teaching and learning requires careful establishment of goals and objectives for a course. Although most instructors do not distinguish between goals and objectives and even dictionaries define each term by the other, in teaching these terms are distinct. Broadly stated, a goal is the overarching aim of instruction, what we intend for the students. For example, one goal in physical chemistry is to provide students with deeper understanding of the mathematical models used by chemists. Objectives are the more specific learning outcomes of instruction and study. Objectives are measurable; we assess student achievements through objectives. Objectives are associated with action words describing what students can do after they have learned that portion of course content. These action words include: draw, derive, explain, calculate, discuss, compare and contrast, etc. A quantum chemistry objective might be “Students will be able to explain the relative wave lengths of the absorption maxima for a series of dyes using the particle in a box model.” Naturally not every instructor uses the same terms to represent what we call goals and objectives. Sometimes objectives are

Table 1. Thermochemistry Goals and Objectives

Goals	Objectives	Tasks
• Review physics and general chemistry fundamental concepts.	• Explain the concepts C_V and C_P with appropriate examples. • Compute the equilibrium temperature when two materials are in contact • Describe the law of conservation of energy in terms of constant volume and constant pressure processes.	• Read the text and answer the questions in the reading guide. • Do assigned problems to assure mastery of these techniques.
• Increase familiarity with the use of tables of thermodynamic data. Increase graph interpretation skills. • Understand the energy requirements for heating a pure substance.	• Recognize and interpret phase changes in C_V and C_P versus T graphs. • Compute the ΔH and ΔU for heating a pure substance when no phase change occurs or when one occurs. • Compute ΔH for a reaction at 298K	• Write answers to assigned questions, compare results with others in your group, and develop consensus for answers to present to the class. • Study assigned graphs, identify phase changes, and compare C_P for different phases. • Do the assigned problems. Work to mastery. Check answers and methods with other members of your group.
• Increase familiarity with computer algebra tool.	• Fit C_P or C_V values for a specific temperature range to a polynomial.	• Apply nonlinear curve fitting techniques. • Apply appropriate statistical measures.
• Appreciate ΔH as a state function. • Understand Hess's Law.	• Compute ΔH for heating a substance when C_P is given as a polynomial function of T or as some other function of T. • Use cyclic diagrams to represent ΔH changes in a system.	• Identify two functions giving C_P as a function of T. What criteria determines when each is used? • Complete problems assigned. Work to mastery. • Identify and annotate sites of potential solution error.
• Use tabulated thermodynamic data to compute ΔH for any reaction at any temperature.	• Distinguish among the various types of ΔH found in published tables.	• Compute $\Delta_{rxn}H(298\ K)$ for the reactions indicated. Work to mastery. • Use the supplied Mathcad template and database to compute $\Delta_{rxn}H(298)$ for several reactions. • Compute $\Delta_{rxn}H(800\ K)$for the NH_3 synthesis. • Extend this template to compute $\Delta_{rxn}H(T)$ for the synthesis of NH_3 at any T.

called performance criteria or instructional outcomes. Sometimes goals are called objectives; however, no matter what word is used the message is clear. Faculty want students to learn certain things and for students to demonstrate learning by doing certain things. It is the faculty who set up the situation by which students can learn and demonstrate that they have learned. Table 1 contains a sample set of goals and objectives for a physical chemistry lesson on thermochemistry.

e. Are we Successful? Three different mechanisms should be used to measure the success of an instructional methodology. First, there is ongoing assessment of the methodology with respect to meeting the instructor's goals. The second asks if the instructor sets the evaluation of students' achievement to match the curriculum's learning objectives. This category contains the exams and student laboratory reports. The third mechanism is the course evaluation where students relate their experiences in the course and how effective they perceived the instruction has been. A caveat is that most course evaluation questions are geared to traditional lecture instruction format. In addition, because students are most familiar with lecture and not in a position to evaluate the learning levels achieved in untraditional class formats, it is important that faculty fine-tune their course evaluation instrument to the course pedagogy.

f. Assessment. Assessing teaching/learning effectiveness involves more than exams and course evaluations. First, assessment and evaluation are different. Assessment is a process whereby an activity's effectiveness is studied. It is formative in that it helps modify practices in light of an ongoing process. Assessment does not provide grades; it provides information for navigational course corrections leading to more effective learning. For example, if an instructor notices that students do not understand a lesson, the instructor can stop and review or ask students to write about what is not being understood. The teacher uses that information to modify the lecture or class activity based on student input. The difficulty is that time is lost, the lecture interrupted, and material covered decreased. The rebuttal asks, of what benefit is covering material when students do not understand what is being said. It is better to cover less, work for deeper understanding of fundamental concepts, and promote long-term fusing of new ideas onto the student's conceptual framework. In addition, time spent helping students to reason through an issue develops their intellectual processing skills so that they will become better independent learners and achieve long-term retention of concepts and skills. One thing that will help teachers to enhance learning is time spent at the beginning of a topic determining the current level of understanding achieved by students. Doing so provides an ideal opportunity for opening the classroom dialogue leading to increased communication and learning.

g. Evaluating Student Learning. Evaluation is the process of judging how much students have learned. Students are primarily evaluated using exams, laboratory reports, research papers, oral presentations, and observed laboratory skills. Some faculty may use student portfolios to measure accomplishment, while others may give oral exams or include selfevaluation when determining final grades.

This leads to several important areas of discussion. First, consider the laboratory where the primary evaluation method is student reports. These reports can be lengthy, containing 10 or more pages of text and data analysis. In a one-credit course with 8 or more experiments, 80 pages of written work are graded. It is no surprise that the physical chemistry laboratory is often designated as a department's writing-intensive course. This output might even be augmented by required oral presentations of the written reports. This scenario is unnecessary and burdensome; fewer reports may result in learning more concepts.

Some suggestions include limiting the number of experiments to five per credit hour. Having some experiments extend over two or three weeks gives the students experience with multiconcept and multistep processes, while techniques requiring concept integration into a single laboratory report mirrors what mature chemists do. There also needs to be a greater overlap of experiments with lecture topics to reduce the burden on students. Occasionally it is impossible to avoid putting concept instruction in the laboratory first; however, when a topic is well developed in the laboratory, the lecture time on the topic should be reduced. Placing practice with symbolic software and molecular modeling at the beginning of the laboratory sequence gives time for lecture to develop to the point where laboratory and lecture are better synchronized.

The primary classroom evaluation method is examinations. Midterm exams usually cover topics from several weeks' instruction. On each exam students are expected to correctly answer several questions ranging from simple computations to memorized or adapted derivations. Interestingly, chemistry students do not score well on physical chemistry exams, even when asked to reproduce an example from class or homework. Is this outcome due to willful neglect, inadequate instruction, or some other factor [112]? Students seem to understand what is done at the chalkboard and can even do the same under our supervision. What is going on here? What may be happening is a form of the "Feynman Effect." Students are very comfortable and enjoy good lectures. They feel that learning has occurred because they understand what the teacher is presenting; however, when alone and struggling with homework or a report, they discover that they cannot reproduce what the teacher has done in class. They are hobbled by lack of practice or experience with the concepts. More lectures will not help. What is needed is a paradigm shift from teacher-centered to student-centered instruction designed to increase student skills for studying the physical chemistry concepts.

First, to help students learn, instructors must clarify the goals and objectives for the course and each lesson within the course. These goals and objectives should be written and shared with students as in Table 1. Students also need to be reminded of the skills required for a lesson. While experienced learners know how to make their own lists of objectives, many students do not have this skill. We best serve our students' needs by providing them with objectives leading them to the stage where they can create the objectives based on our lecture or assigned work. Furthermore, students should be able to study some sections of physical chemistry independently by analyzing the material themselves and identifying goals and objectives for that material.

After completing a lesson using clearly delineated goals and objectives, students should know precisely what to expect on a test. They can work to master the skills specified in the objectives by homework, by studying examples from various available texts, or group work with classmates. The instructor has a clear responsibility to focus on the objectives when constructing an exam. An exam's purpose is to determine what a student has learned and not what the best students might be able to figure out during one hour of concentrated effort. One measure of success in matching exam quality with student performance is that a hard working average student should be able to achieve a score of C on an absolute scale. Exam scores with means in the 20% to 40% range are ineffective evaluation tools. They are unlikely to help the instructor modify instruction or help the students to work toward better performance. Scores this low require application of curves when assigning final letter grades to students. Such grading does not discriminate among students with varying levels of achievement. Students also learn quickly to triage their studying. If increased studying does not pay off with increased scores, students are more likely to settle for a C or D on a curve to complete the chemistry major rather than to strive for excellence in understanding. This attitude does not bode well for the chemical profession or the perceptions transmitted to future generations of students.

Another method of evaluation is the ACS DivCHED standardized examination in physical chemistry. The director of the ACS DivCHED Examinations Institute typically chooses the committee chairperson, a scientist actively engaged in physical chemistry research and teaching, who then selects physical chemists to construct this exam. The committee members are chosen based on a distribution reflecting the size and geographical location of schools and area of expertise [113]. All members of the committee are volunteers.

The goal of the exam committee is to design exams based on a set of criteria, including audience, major, and topics. Audiences include schools providing physical chemistry instruction primarily to engineering students, chemistry majors, biology majors, etc. The exams do not require instructors to teach the same topics. Since the exam covers a broad spectrum of topics, it is possible that up to 20% of the questions on a particular exam may not have been covered in an individual physical chemistry course. Consequently it is futile to use the results of ACS exams to determine the quality of instruction. To do so encourages faculty to teach to the exam, although the bulk of the topics represented on the examination should be covered. The ACS CPT also provides a list of topics [13] albeit leaning toward an older curriculum. A good selection of content could be chosen from either topic source.

Physical chemistry exams are nationally normed using up to 500 or more student exams. In some cases, such as the physical chemistry comprehensive form, as few as 200 student exams may be used for the norms. There are both disadvantages and advantages to using normed rather than standards-based exams. First, norming data depend on individual instructors reporting student data to the Examinations Institute. This may make it difficult to obtain norms representative of a various teaching environments and student achievement levels. Nevertheless, a good comparison of one group of students to a large group of students from across a broad spectrum of teaching environments is obtained. The most important advantage is that committee construction eliminates the biases introduced by a single author/instructor and because the exams are thoroughly proofread and checked, there is minimal error. Each physical chemistry exam suite takes approximately five years to develop and norm. The nature of the physical chemistry exams has changed over the past 20 years. These changes reflect the evolution of the discipline in topics and their weighting, in teaching and assessment strategies, in style of production, and in student technological sophistication. The advent of signal-sending calculators has moved the exam to a format excluding the use of calculators. This is pushing the nature of the exam into a more conceptual mode, one in which interpretation of graphics and fundamental understanding of concepts is emphasized. The committee also works to create a balanced exam smoothly transitioning from older topics to newer topics over the years. In this way the committee provides a small amount of pressure to drive modernization of the curriculum.

h. Qualitative versus Quantitative Assessment. One of the important tenets of recent chemical education research is a paradigm shift from examining what is presented to students to an understanding of what students have learned. Examinations and laboratory reports provide one point of measurement of this learning. Another source of information is a structured, or free form, interview about specific topics. Such interviews focus on a problem presented to a student, and that student's method(s) of solution in an environment where discussions with an interviewer are taped [114, 115]. Surveys [116, 117] and student writing [118] provide additional mechanisms for discerning more about student conceptions. A newer technique analyzes student written communications from archived discussions made using course software during intercollegiate or intracollegiate projects. Such analysis creates a map of student interaction frequency and fluency. This coupled with analysis of message content reveals levels of understanding that are impossible to detect using traditional exams [119].

7. Critical Issues

a. Presenting What Physical Chemists Do Today. The excitement of doing physical chemistry research is reflected in the areas of study published by practicing physical chemists, not by the historical accomplishments of Ostwald and others [6].

b. At and Beyond the Basics. The chemistry curriculum requires that we provide instruction on the physical chemistry concepts underpinning the work of all chemists. How is this breadth of conceptual knowledge to be learned? Should we focus on presentation of concepts in the standard mode that we are all used to? Or do we invent new ways of transmitting those concepts by imbedding them in relevant chemical contexts? We contend that it is more likely for students to learn and retain core concepts when they are placed in the rich environment of modern physical chemistry research topics. While substantial amounts of time should be used to portray fundamental concepts as applied to modern chemical problems, care must be taken to not create a false comfort zone for students who may learn the context but not have a firm grasp of the concepts. A balance is required when using context as the stepping stone to firm concept learning. This allows students to see the excitement of current research in chemistry and the necessity of understanding physical chemistry well. There should also be a greater emphasis on biochemical applications of physical chemistry concepts and methods. Many of the most fascinating scientific problems arising for the current and future generations of chemistry students will involve biochemistry. Most science majors today are in biology or biochemistry programs. There is also a need to link to other disciplines such as materials science.

c. Using Technology. It is impossible to imagine teaching physical chemistry without instruments or computers [120]. First, computers should be used for data acquisition in all experiments in the laboratory. Recording data by hand is time consuming, subject to recording error, and a waste of valuable student-learning time. Fortunately, most instruments come computer-interfaced or ready to connect to computers. Following data acquisition, all students must be fluent with data reduction, all reports must be prepared using word processing software, and rules previously applied to hand-drawn plots must be used in preparing digital data plots.

When teaching physical chemistry, instructors should use computers in the classroom. A tool such as PowerPoint may be useful, but spreadsheets and symbolic algebra software are more powerful. When used in the classroom, these tools provide ways to do live computation on large data sets not possible with chalk or pencil and paper. Animation or display and modification of mathematical functions help students to see relationships and to appreciate and become comfortable with them. Better yet is to have students use the same software while providing them with guided-inquiry activities for exploration and construction of a solid understanding of a topic. Ample resources exist for using symbolic algebra in physical chemistry. Mathematica users have a number of book and electronic resources [121, 122] as do Maple users [123, 124]. The most useful resources, however, may be the Mathcad collection [125], the growing national digital library of chemistry resources [126], and books including Mathcad exercises or examples for physical chemistry [127, 128]. Because typing symbolic algebra files or worksheets and large data sets is very time-consuming, it is best for students to use faculty-developed templates and data files. This permits students to focus their time on fruitful exploration of concepts rather than frustrating typing and debugging activities.

Besides symbolic algebra software, students should also have good skills with spreadsheets or a program such as Sigma Plot, PsiPlot, etc. Strength with laboratory data analysis software can offset less skill with symbolic algebra software. Carefully constructed spreadsheets or symbolic algebra exercises are persuasive tools for enhancing learning of mathematical models in physical chemistry courses.

Another skill for the physical chemistry student is familiarity with computational chemistry software. All chemistry students should be able to prepare structures for visual display of molecular shapes and to perform quantum chemistry calculations to determine molecular properties. Students should know, through software use, the core concepts behind semi-empirical, ab initio, and molecular mechanics/dynamics calculations. These skills need to be integrated throughout the curriculum, but their mathematical foundations should be found in the physical chemistry course. After completing physical chemistry, students should be able to describe a basis set and distinguish between ab initio and semi-empirical calculations. They should understand the outline of the structure of these computational approaches. This does not imply that students need to be computational chemists, but rather that they should be well on their way to being wise consumers of computational chemistry results.

Some may still think that skill in writing code in Basic, Fortran, or C is essential. We do not think so. Physical chemists developing software can learn programming skills outside the chemistry curriculum. Logical thinking and precision of expression are equally well-taught through symbolic algebra and spreadsheet software. The chemistry student may not even need to write code for collection of data from an instrument. In any case, those needing to learn this level of code writing will benefit from experiences with symbolic or spreadsheet software.

The computer is an essential communication tool. Not only must the student write reports, but they should also be able to search for, retrieve, and evaluate chemical information from many sources. They must be able to communicate with other chemists via discussion forums. Because students are usually reluctant to use computers for communication about science, they remain consumers of information presented in lecture; however, they will be expected to share expertise and to communicate effectively with others in various professional settings. An excellent way to enhance the communication skills of students is to have them participate in projects requiring significant online interaction with other students in their classes or across campuses.

Intra- and intercollegiate activities have been the focus of the Physical Chemistry Online community for the past seven years [129]. Through this project physical chemistry students explore both old and new topics in chemistry. These topics come from the standard repertoire or newly created context-rich materials. In these projects, students perform experiments while interacting with other students from distant campuses to share data and discuss scientific concepts. The most difficult aspects have proven to be promoting communication among students and the participatory work for the faculty facilitator [109, 119, 130, 131].

In addition to mathematical modeling and computational chemistry packages, other technology-based resources are available. The World Wide Web provides many different kinds of pedagogical and scientific resources for the technology-uninhibited. Commercial publishers are also beginning to distribute their own versions of MathCAD™ templates [127, 132] or collections [133]. In the future, we see DVDs featuring modern physical chemistry topics that instructors can use in courses. In one such project, an interactive Web-enhanced DVD is being produced featuring a discussion of applications of modern physical chemistry, interviews with the scientists performing the experiments, background material, sample data from the experiments, and structured questions about the theory, the experiment, and the sample results. The DVD emphasizes the practical aspects of physical chemistry in medical, environmental, and other contexts that students can relate to and uses an interface that accommodates students with different learning styles. The first modules are nearing completion, with the complete set of 10 modules scheduled for late 2005 [134]. Another future resource is a physical chemistry ebook [135] incorporating images, multimedia components, and symbolic algebra activities.

8. Conclusion

Given the nature of the specialization called physical chemistry, it is difficult to provide a uniform standard for a curriculum driven by the diverse interests of physical chemists and the demands for physical chemistry expertise required by a broad range of interdisciplinary scientific questions. At best we can only offer guidelines for the teachers of this critical undergraduate curriculum component. These guidelines are that physical chemistry should:

Reflect what physical chemists do today

(a) Present essential core concepts for the vast majority of students in the class who will not be physical chemists
(b) Enrich core concepts with significant modern examples from the literature
(c) Significantly increase the opportunities for interpreting data and applying models to data
(d) Make optimal use of information technology and computer resources
(e) Use sound pedagogical practices to enhance learning and development of critical interdisciplinary skills in students.

Graduate student instruction should further probe the models used by modern physical chemists while extending the expertise of the graduate chemist to using fundamental physical chemistry concepts in a broad range of interdisciplinary activities with deeper understanding and skill. All chemistry graduate students should explore one or more specialized areas of physical chemistry. Physical chemistry graduate students should have advanced training in quantum chemistry, molecular modeling, chemical dynamics, thermodynamics, and spectroscopy in addition to their Ph.D. thesis work. Studying physical chemistry should provide students with the tools to be able to pursue additional independent study in their own field and allied fields as required for competence in the discipline and flexibility of scholarship.

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References and Notes

1. Pignataro, S. *La Chimica e l'Industria* **1998,** *80,* 1282–1284.
2. Glasstone, S. *Textbook of Physical Chemistry,* 2nd ed.; D. Van Nostrand Co. Inc.: New York, 1946.
3. Atkins, P.; dePaula, J. *Physical Chemistry,* 7 ed.; W. H. Freeman and Company: New York, 2002.
4. Berry, R. S.; Rice, S. A.; Ross, J. *Physical Chemistry,* 2nd ed.; Oxford University Press: New York, 2000.
5. McQuarrie, D. A.; Simon, J. D. *Physical Chemistry: A Molecular Approach;* University Science Books: Sausalito, CA, 1997.
6. Servos, J. W. *Physical Chemistry from Ostwald to Pauling;* Princeton University Press: Princeton, NJ, 1990.
7. Daniels, F. *J. Chem. Educ.* **1958,** *35,* 322–333.
8. Cartledge, G. H. *J. Chem. Educ.* **1924,** *1,* 119–127.
9. *Content of Undergraduate Physical Chemistry Courses*, American Chemical Society: Washington DC, 1984.
10. Lippincott, W. T., Ed. *Essays in Physical Chemistry;* American Chemical Society: Washington, DC, 1988.
11. Moore, R. J.; Schwenz, R. W. *J. Chem. Educ.* **1992,** *69,* 1001–1002.
12. Schwenz, R. W.; Moore, R. J. *Physical Chemistry: Developing a Dynamic Curriculum;* American Chemical Society: Washington DC, 1993.
13. American Chemical Society 2004. http://www.chemistry.org/portal/a/c/s/1/acsdisplay.html?DOC=education\cpt\ts_physchem.html (accessed Feb 2004).
14. New Traditions Physical Chemistry Curriculum Planning Group 1995. http://newtraditions.chem.wisc.edu/PRBACK/pchem.htm (accessed Feb 2004).
15. PolymerCoreCourseCommittee *J. Chem. Educ.* **1985,** *62,* 780.
16. PolymerCoreCourseCommittee *J. Chem. Educ.* **1985,** *62,* 1030.
17. White, M. A. *Properties of Materials;* Oxford University Press: New York, 1999.
18. Ellis, A. B.; Geselbracht, M. J.; Johnson, B. J.; Lisensky, G. C.; Robinson, W. R. *Teaching General Chemistry: A Materials Science Companion;* American Chemical Society: Washington, DC, 1993.
19. Ellis, A. B. *J. Chem. Educ.* **1997,** *74,* 1033–1039.
20. Cramer, C. J. *Essentials of Computational Chemistry: Theories and Models;* Wiley: New York, 2002.
21. Shea, J.-E.; Brooks II, C. L. *Ann. Rev. Phys. Chem* **2001,** *52,* 449–535.
22. Liu, K. *Ann Rev Phys Chem* **2001,** *52,* 139–164.
23. Tropsha, A.; Bowen, J. P. In *Using Computers in Chemistry and Chemical Education;* Zielinski, T. J.; Swift, M. L., Eds.; American Chemical Society: Washington DC, 1997, pp 309–330.
24. Northrup, S. H. In *Using Computers in Chemistry and Chemical Education;* Zielinski, T. J., Swift, M. L., Eds.; American Chemical Society: Washington DC, 1997, pp 283–308.
25. Ladanyi, B. M. In *Theoretical Methods of Condensed-Phase Chemistry;* Schwartz, S. D., Ed.; Kluwer: Dordrecht, 2000, pp 207–233.
26. Zewail, A. H. *Femtochemistry—Ultrafast Dynamics of The Chemical Bond,* Vols. I and II; World Scientific: Singapore, 1994.
27. McCash, E. M. *Surface Chemistry;* Oxford University Press: Oxford, 2001.
28. Shinar, J.; Vardeny, Z. V.; Kafafi, Z. H., Eds. *Optical and Electronic Properties of Fullerenes and Fullerene-Based Materials;* M. Dekker: New York, 2000.
29. JILA BEC Homepage. http://jilawww.colorado.edu/bec/ (accessed Feb 2004)
30. Finlayson-Pitts, B. J.; James N. Pitts, J. *Chemistry of the Upper and Lower Atmosphere: Theory, Experiments, and Applications;* Academic: San Diego, 2000.
31. Hinsberg, W. D.; Wallraff, G.; Houle, F. A.; Morrison, M.; Frommer, J.; Beyers, R.; Hutchinson, J. In *Organic Thin Films;* Frank, C., Ed.; American Chemical Society: Washington DC, 1998, pp 344–359.
32. Ott, J. B.; Boerio-Goates, J. *Chemical Thermodynamics: Advanced Applications;* Academic Press: New York, 2000; Vol. II.
33. Kastner, M. E.; Vasbinder, E.; Kowalcyzk, D.; Jackson, S.; Giammalvo, J.; Braun, J.; DiMarco, K. *J. Chem. Educ.* **2000,** *77,* 1247–1248.
34. Rhodes, G. *Crystallography Made Crystal Clear: A Guide for Users of Macromolecular Models,* 2 ed.; Academic: San Diego, CA, 2000.
35. Karplus, M.; McCammon, J. A. *Nature Struct. Biol.* **2002,** *9,* 646–652.
36. Gao, J. *Acc. Chem. Res.* **1996,** *29,* 298–305.
37. Bodner, G. M. *J. Chem. Educ.* **1987,** *64,* 513–514.
38. Frank, D. V.; Baker, C. A.; Herron, J. D. *J. Chem. Educ.* **1987,** *64,* 514-515.
39. Bunce, D.; Heikkinen, H. *J. Res. Sci. Teach.* **1986,** *23,* 11–20.
40. Arons, A. B. *Liberal Education* **1985,** *71,* 141–158.
41. Pople, J. A. *Rev. Mod. Phys.* **1999,** *71,* 1267–1274.
42. Hinsber, W.; Houle, F. http://www.almaden.ibm.com/st/computational_science/ck/msim/?overview (accessed Feb 2004).
43. Johnstone, R. A. W.; Rose, M. E. *Mass Spectrometry for Chemists and Biochemists;* Cambridge University Press: New York, 1996.
44. Tinoco, I., Jr.; Sauer, K.; Wang, J. C.; Puglisi, J. D. *Physical Chemistry: Principles and Applications in Biological Sciences,* 4th ed.; Prentice Hall: Upper Saddle River, NJ, 2002.
45. Bergethon, P. R. *The Physical Basis of Biochemistry;* Springer-Verlag: New York, 1998.
46. Daniels, F. *Mathematical Preparation for Physical Chemistry*; McGraw Hill: New York, 1928.
47. Daniels, F. *J. Chem. Educ.* **1929,** *6,* 254–259.
48. Francl, M. *Survival Guide for Physical Chemistry;* Physics Curriculum & Instruction: Lakeville, MN, 2001.
49. Craig, N. C. *J. Chem. Educ.* **2001,** *78,* 582–586.
50. Topper, R. Q.; Freeman, D. L.; Bergin, D.; LaMarche, K. In *Reviews in Computational Chemistry;* Lipkowitz, K. B.; Larter, R.; Cundari, T., Eds.; John Wiley and Sons: New York, 2003; Vol. 19, in press.
51. Ganter, S. L. *Changing Calculus: A Report on Evaluation Efforts and National Impact from 1988–1998*. The Mathematics Association of America, 2001.
52. Grushow, A.; Zielinski, T. J. *J. Chem. Educ.* **2002,** *79,* 707–714.
53. DeGraff, B. A.; Hennip, M.; Jones, J. M.; Salter, C.; Schaertel, S. A. *Chem. Educator* **2002,** *7,* 15–18; DOI 10.1333/s00897020531a.
54. Lorigan, G. A.; Patterson, B. M.; Sommer, A. J.; Danielson, N. D. *J. Chem. Educ.* **2002,** *79,* 1264–1266.
55. Hodgson, S. C.; Bigger, S. W.; Billingham, N. C. *J. Chem. Educ.* **2001,** *78,* 555–556.
56. Garland, C. W.; Nibler, J. W.; Shoemaker, D. P. In *Experiments in Physical Chemistry,* 7th ed.; McGraw-Hill: Boston, 2003, pp 328–335.
57. Akins, D. A.; Bailey, R. A.; Giachino, G. B.; Moore, J. A.; Tomkins, T. P. T. In *Integrated Experimental Chemistry: Principles and Techniques;* Allyn and Bacon: New York, 1978; Vol. 2.
58. Kutz, H. D.; Copeland, J. H.; Mathai, G. T. C. *J. Chem. Educ. Software* **2003,** *80,* 106.
59. Lacks, D. R. D. *J. Chem. Educ. Software* **2003,** *4C2.*
60. Grushow, A. *J. Chem. Educ.* **2000,** *77,* 1527.
61. Foresman, J. B.; Frisch, A. *Exploring Chemistry with Electronic Structure Methods,* 2nd ed.; Gaussian: Pittsburgh, 1996.

62. Hehre, W. J.; Radom, L.; Schlyer, P. V. R.; Pople, J. A. *Ab Initio Molecular Orbital Theory;* Wiley: New York, 1986.
63. Caffery, M. L.; Dobosh, P. A.; Richardson, D. M. *Laboratory Exercises using Hyperchem;* Hypercube: Gainesville, Florida, 1998.
64. Foresman, J. B. In *Using Computers in Chemistry and Chemical Education;* Zielinski, T. J., Swift, M. L., Eds.; American Chemical Society: Washington DC, 1997, pp 243–256.
65. Hehre, W. J. In *Using Computers in Chemistry and Chemical Education;* Zielinski, T. J.; Swift, M. L., Eds.; American Chemical Society: Washington DC, 1997, pp 257–281.
66. Wong, C.; Currie, J., Eds. *Teaching with CAChe: Exercises on Molecular Modeling in Chemistry;* Fujitsu Limited: Beaverton, OR, 2001.
67. Ellison, M. D. *J. Chem. Educ.* **2003,** *80,* 581.
68. Zielinski, T. J.; Shalhoub, G. M. *J. Chem. Educ.* **1998,** *75,* 1192.
69. Zielinski, T. J. *J. Chem. Educ.* **1998,** *75,* 1191.
70. Wright, J. C.; Zielinski, T. J. *J. Chem. Educ.* **1999,** *76,* 1367–1373.
71. Shalhoub, G. M.; Zielinski, T. J. *J. Chem. Educ.* **1998,** *75,* 1192.
72. Valero, M.; Rodriguez, L. J.; Velázquez, M. M. *J. Chem. Educ.* **1999,** *76,* 418.
73. Crane, N. J.; Mayrhofer, R. C.; Betts, T. A.; Baker, G. A. *J. Chem. Educ.* **2002,** *79,* 1261.
74. Zielinski, T. J.; Grushow, A.; Shalhoub, G. 2002. http://bluehawk.monmouth.edu/~tzielins/PCOLWEB/Cyclodextrin2002/. (accessed Feb 2004).
75. Ticich, T. M. In *Physical Chemistry: Developing a Dynamic Curriculum;* Schwenz, R. W., Moore, R. J., Eds.; American Chemical Society: Washington, DC, 1993, pp 462–470.
76. Whisnant, D. M.; Howe, J. J.; Lever, L. S. *J. Chem. Educ.* **2000,** *77,* 199–201.
77. Harvey, E.; Sweeney, R. *J. Chem. Educ.* **1999,** *76,* 1309.
78. Harvey, E.; Sweeney, R. *J. Chem. Educ.* **1999,** *76,* 1310.
79. Whisnant, D. M.; Lever, L. S.; Howe, J. J. *J. Chem. Educ.* **2000,** *77,* 1648.
80. Wavefunction. http://www.wavefunction.com/ (accessed Feb 2004).
81. Gaussian Inc. http://www.gaussian.com/ (accessed Feb 2004).
82. Mathcad.Mathsoft Inc. http://www.mathcad.com/ (accessed Feb 2004).
83. Maplesoft. http://www.maplesoft.com/ (accessed Feb 2004).
84. Mathematica. http://www.wolfram.com/ (accessed Feb 2004).
85. Bodner, G. M. *J. Chem. Educ.* **1986,** *63,* 873.
86. Bodner, G. M. *J. Chem. Educ.* **1991,** *68,* 385–388.
87. Chinn, C. A.; Brewer, W. F. *Rev. Educ. Res.* **1993,** *63,* 1–49.
88. Herron, D. J. *J. Chem. Educ.* **1975,** *52,* 146.
89. Bloom, B. S., Ed. *Taxonomy of Educational Objectives: The Classification of Educational Goals;* D. McKay: NY, 1956.
90. Perry, W. G., Jr. *Forms of Intellectual Development in the College Years: A Scheme;* Holt Rinehart, and Winston: New York, 1970.
91. King, P. M.; Kitchener, K. S. *Developing Reflective Judgment: Understanding and Promoting Intellectual Growth and Critical Thinking in Adolescents and Adults;* Jossey-Bass: San Francisco, 1994.
92. Paul, R. *Critical Thinking—What Every Person Needs to Survive in a Rapidly Changing World,* Revised 2nd ed.; The Foundation for Critical Thinking: Santa Rosa, CA, 1992.
93. Shulman, L. S. *Educational Researcher* **1986,** *15,* 4–14.
94. Herron, J. D. *The Chemistry Classroom: Formulas for Successful Teaching;* American Chemical Society: Washington, DC, 1996.
95. Hestenes, D.; Wells, M.; Swackhamer, G. *Physics Teacher* **1992,** *30,* 141–158.
96. Hestenes, D. H.; Halloun, I. *Physics Teacher* **1995,** *33,* 502.
97. Hayes, J. *The Complete Problem Solver;* Erlbaum: Hillsdale NJ, 1981.
98. Belenky, M. F.; Clinchy, B. M.; Goldberger, N. R.; Tarule, J. M. *Women's Ways of Knowing—The Development of Self, Voice, and Mind;* Basic Books, Inc., 1986.
99. Finster, D. C. *J. Chem. Educ.* **1989,** *66,* 659–661.
100. Finster, D. C. *J. Chem. Educ.* **1991,** *68,* 752–756.
101. Welfel, E. J. *J. Coll. Stu. Pers.* **1982,** *23,* 490–497.
102. Zoller, U. *J. Chem. Educ.* **1987,** *64,* 510.
103. Angelo, T. A.; Cross, K. P. *Classroom Assessment Techniques,* 2nd ed.; Jossey-Bass Publishers: San Francisco, 1993.
104. Johnson, D. W.; Johnson, R. T.; Smith, K. A. *Active Learning: Cooperation in the College Classroom;* Interaction Book Co.: Edina, MN, 1991.
105. Felder, R. M. *J. Chem. Educ.* **1996,** *73,* 832–836.
106. Spencer, J.; Moog, R. S.; Farrell, J. J. *Physical Chemistry: A Guided Inqiry—Thermodynamics,* 1st ed.; Houghton Mifflin, 2004.
107. Moog, R. S.; Spencer, J. N.; Farrell, J. J. *Physical Chemistry: A Guided Inqiry—Atoms, Molecules, and Spectroscopy,* 1 st ed.; Houghton Mifflin: New York, 2004.
108. Duncan-Hewitt, W.; Mount, D. L.; Apple, D. *A Handbook on Cooperative Learning,* 2nd ed.; Pacific Crest: Corvallis, OR, 1995.
109. Towns, M.; Sauder, D.; Whisnant, D.; Zielinski, T. J. *J. Chem. Educ.* **2001,** *78,* 414.
110. Sauder, D.; Towns, M.; Derrick, B.; Grushow, A.; Kalow, M.; Long, G.; Miles, D.; Shalhoub, G.; Stout, R.; Vaksman, M.; Pfeiffer, W.; Weaver, G.; Zielinski, T. J. *Chem. Educator* **2000,** *5,* 77–82; DOI 10.1333/s00897000369a.
111. Ricci, R. W.; Van Doren, J. M. *J. Chem. Educ.* **1997,** *74,* 1372.
112. Zielinski, T. J.; Brooks, D. W.; Crippen, K. J.; March, J. L. *J. Chem. Educ.* **2001,** *78,* 714–715.
113. Holme, T. *J. Chem. Educ.* **2003,** *80,* 594–596.
114. Thomas, P. L.; Schwenz, R. W. *J. Res. Sci. Teach.* **1998,** *35,* 1151.
115. Lang, P. L.; Towns, M. H. *J. Chem. Educ.* **1998,** *75,* 506.
116. Nicoll, G.; Francisco, J. S. *J. Chem. Educ.* **2001,** *78,* 99.
117. Patron, F. In *Chemistry*; Purdue University: West Lafayette, IN, 1997.
118. Beall, H. *J. Chem. Educ.* **1994,** *71,* 1056.
119. Slocum, L. E.; Towns, M. H.; Zielinski, T. J. *J. Chem. Educ.*; in press.
120. Zielinski, T. J.; Swift, M. L. *Chem. Educator* **1997,** *2*(3); S1430-4171(97)03124-5; DOI 10.1333/s00897970124a
121. Cropper, W. H. *Mathematica Computer Programs for Physical Chemistry;* Springer: New York, 1998.
122. Francl, M. M. Mathematica Information Center 2000. *Introduction to Statistical Mechanics*. http://library.wolfram.com/infocenter/MathSource/814 (accessed Feb 2004).
123. Scarlete, M.1998. *WWW Living-Book of Physical Chemistry (CD-ROM version).* http://chemlog.ubishops.ca/newserie/toc.htm (accessed Feb 2004).
124. http://www.maplesoft.com/publications/books/indexby/category/Chemistry.shtml (accessed Feb 2004).
125. Zielinski, T. J. 2003. Mathcad Documents for Physical Chemistry. http://bluehawk.monmouth.edu/~tzielins/mathcad/index.htm (accessed Feb 2004).
126. NSDL. Journal of Chemical Education National Science Digital Library Collection. http://jce.divched.org/JCEDLib/ (accessed Feb 2004).
127. Cady, M. P.; Trapp, C. A. *A Mathcad Primer for Physical Chemistry;* W. H. Freeman and Company: New York, 2000.
128. Noggle, J. H. *Physical Chemistry Using Mathcad;* Pike Creek Publishing: Newark, DE, 1997.
129. PCOL. http://pcol.ch.iup.edu/ (accessed Feb 2004).

130. Towns, M. H.; Kreke, K.; Fields, A. *J. Chem. Educ* **2000,** *77,* 111.

131. Towns, M. H.; Kreke, K.; Sauder, D.; Stout, R.; Long, G.; Zielinski, T. J. *J. Chem. Educ.* **1998,** *75,* 1653.

132. Atkins, P.; dePaula, J. *Explorations in Physical Chemistry: A Resource for Users of Mathcad;* WH Freeman: New York, 2002.

133. Holmes, Jon L.; Gettys, Nancy S. *J. Chem. Educ.* **2003** *80* 1222 http://jchemed.chem.wisc.edu/JCESoft/Programs/ACC/index.html (accessed Mar 2004).

134. Weaver, G. C., Physical Chemistry in Practice, DVD. This DVD can be obtained from Gabriela Weaver the author. Purdue University, Department of Chemistry, 560 Oval Drive, West Lafayette, IN 47907-2084.

135. Hanson, D. M.; Harvey, E.; Sweeney, R.; Zielinski, T. J. 2003. Quantum States of Atoms and Molecules. http://bluehawk.monmouth.edu/~tzielins/QuantumStates/index.htm (accessed Feb 2004); beta version available from the authors.