Exploring Quantum Concepts in Chemistry:

Active Discovery by Students in the General Chemistry Course

I. Rationale for the Project

General chemistry is a core course for students considering careers in the natural sciences, engineering, medicine, or other technology fields. It is also a critical course for the preparation of an informed 21st Century citizenry to understand the public policy issues of the impact of technology upon society and the environment. The large number of students who take general chemistry makes the content of this course of great importance to the quality of undergraduate education nationally. The relevance and accessibility of the material in the general chemistry course affects many students' career decisions. Our nation has an economic imperative to train workers for jobs in biotechnology, advanced medical care, the computer and electronics industries, and in the materials sciences. In general, there is a need to encourage students considering careers in the science and technology fields, and to support their mastery of new concepts in chemistry.

We propose to develop a new approach to the quantum aspects of the general chemistry course taken by undergraduates majoring in the sciences at American colleges. This approach will emphasize the teaching of quantum concepts as the foundation of modern chemistry and science. It relies on three convergent streams of development in the sciences and education: (1) modern science and technology are becoming ever more reliant on our understanding of the quantum nature of matter; (2) educational research has provided us with new insights into how students develop the deep conceptual understanding necessary for the transfer of learning to new domains; and, (3) the interactive control of computer graphics provides for the exploration and visualization of quantum concepts. The first development provides the need and significance of the proposed project. The second provides the justification for the method of instruction and approach we propose. Finally, computer tools provide the vehicle for our project.

Through prior projects and professional activities, the members of the proposed project team are already an integrated unit. We have named an Advisory Board of nationally known and geographically distributed chemistry education experts to broaden the intellectual input to the project, as well as improve the visibility and eventual dissemination of our products. To ensure input from faculty at diverse institutions during the project development, we have arranged for consulting support from the New England Board of Higher Education.

The proposed work is based on a study that involved the use of software tools specifically designed to enable students to explore visually the quantum aspects of atoms and molecules. These tools, developed for the National Science Foundation funded project Quantum Sciences Across Disciplines project (QSAD), provide a route to elucidation and exploration of quantum ideas that bypasses the barriers presented by traditional approaches based on detailed mathematical analysis. With these tools, quantum concepts emerge for the student in a descriptive language of shape, location, and color. Based on this prior experience, we propose to:

- design and implement interactive software for instruction of quantum concepts at a level suitable for science concentrators in general chemistry courses;
- design complementary laboratory experiments for testing of quantum concepts;
- create and disseminate the supporting text for the materials to be learned, and an instructor’s manual documenting effective instructional strategies;
- provide a test bed for the incorporation of new teaching strategies appropriate for medium and large size general chemistry courses using computer software;
- begin to offer annual, self-sustaining workshops in the use of our materials for chemistry instructors from two-year and four-year institutions in the final year of the proposed work.

1. The Need to Introduce Quantum Concepts in Chemistry. The year 2000 marked the 100th anniversary of the quantum model. Quantum concepts now underpin our modern understanding of the universe and our ability to control nature for human needs. The crafts of modern chemistry, materials science, and electrical engineering rely on the manipulation of matter at the atomic and molecular level. This is fast becoming true of biology as well. The products are new technologies and experimental probes: new polymeric materials, new ceramics, new electronics materials including LEDs and microelectronic circuits, new approaches to computation through electronics, coding, and information processing, and new spectroscopies.

This ubiquitous use of the quantum model of matter throughout the sciences and technology will propel it to the center of 21st general chemistry courses. To this end, it is unnecessary to teach the mathematical aspects of quantum chemistry to freshman students. The concepts in the quantum model are few in number, but enormous in consequence. Quantized energy levels, spin, the geometry of electronic orbitals, and the Pauli Principle can all be understood qualitatively and descriptively, and then applied to chemical behavior, extending from the single atom, to small molecules, to polymers, and finally to the properties of materials.

2. Students learn best when provided with the opportunity for active exploration. For the past century quantum theory has been at the heart of modern chemistry just as chemistry is at the heart of materials science and medical research. Nevertheless, instruction at a level that deeply engages students in quantum ideas has been largely avoided in general chemistry due to the belief by instructors that the material is too mathematically abstruse. Our experience is that this barrier can be largely removed by using a discovery-based approach relying on interactive tools for the exploration and visualization of quantum behavior.

Providing in-depth instruction through the use of a fundamental conceptual model is an approach supported by current research on the science of learning. The Committee on Learning Research and Educational Practice of the National Research Council writes “A key finding in the learning and transfer literature is that organizing information into a conceptual framework allows for greater ‘transfer’; that is, it allows the student to apply what was learned in new situations and to learn related information more quickly” (NRC, 1999). The NRC Committee further writes, “To develop competence in an area of inquiry, students must have opportunities to learn with understanding. Deep understanding of subject matter transforms factual information into usable knowledge.”

Our hypothesis is that students provided with well-conceived instruction on the quantum model of chemical behavior will be able to understand better a wide range of chemical properties, spectroscopic techniques, and the behavior of materials.

3. The authentic use of computers for general chemistry education. The use of computers for symbolic and virtual graphical representation is now ubiquitous in chemistry research. In a similar manner, we see computer graphics as essential to providing students insight into modern chemistry and science. We further believe that, properly used, computers can offer innovative solutions to the educational problem of how to teach effectively when the student-professor ratio is high. Problems that benefit from the authentic use of the power of software are ones that require individual interactive exploration of otherwise inaccessible concepts. For example, if merely displaying the electronic distribution associated with an atomic orbital were sufficient, then current texts would do an admirable job in teaching quantum concepts, since they all contain such pictures. In fact, these texts are not successful (Shiland, 1997) because students are not able to understand what is being represented. By contrast, the interactivity of properly designed computer software enables students to explore the meaning of what they are observing by varying controlling parameters. Research for the QSAD project in high schools demonstrated that, to successfully introduce a software-based approach to teaching quantum concepts, teachers had to modify their instructional approach to use the software effectively (Robblee et al, 2000).

II. Project Objectives

Our long-term goal is to devise new instructional techniques to provide general chemistry students with a better and deeper conceptual understanding of the physical world, an understanding that they can transfer to the study of other sciences and technologies, and the knowledge to make informed decisions as citizens. To support this, the scope of the proposed project is specified by our short-term objectives:

Objective 1: ***Create an introduction to the quantum aspects of matter for general chemistry students.*** We propose to develop materials that, when distributed over the term, will occupy about half of a semester in a one-year general chemistry course. These materials will allow students to explore the basis of our modern understanding of atomic and molecular electronic structure, and then to learn how to use this understanding to explain the properties and dynamic behavior of materials. These behaviors include: the continuum of ionic, polar covalent, and covalent bonding; properties of acids and bases as determined by charge distribution; electronegativity; redox reactions; organic synthesis, properties of organic macromolecules of biological interest such as proteins, carbohydrates, and nucleic acids; the properties of inorganic materials such as metals, plastics and ceramics; and the response of such materials to spectroscopic probing with electromagnetic fields. The planned curriculum materials may ultimately be used as a foundation for explaining the remaining topics in the general chemistry sequence.

Objective 2: ***Create software for quantum instruction in general chemistry.*** Modern science relies heavily upon the use of computers for visual realizations of microscopic theories of physical behavior. From these graphical representations arise a descriptive approach with metaphors and similes to describe the atomic and molecular behaviors that give rise to macroscopically observable effects. This project will develop interactive computer software to provide general chemistry students with a visual and descriptive introduction to the different representations of our understanding of atomic and molecular structure. This software will be written in Java for cross-platform use, and be downloadable from the web.

Objective 3: ***Create an instructional environment that supports a deep understanding of the properties of matter.*** Lecturing represents one end of a continuum of instructional strategies. It relies upon a transmission model for student learning: the instructor transmits, the student listens. At the other end of the spectrum, the student is the primary actor who discovers new truths with the assistance of a tutor. The reality of general chemistry instruction at major universities is that the student-professor ratio is too high, and the quantity of material too demanding, for the instructor to provide each student with individual attention. It is our intention to investigate intermediate instructional methods for science courses with large enrollments and to provide a model of how to shift instruction from transmission to personal construction through the use of software for computer-based explorations, peer group collaborative instruction, and assignments designed to stimulate student inquiry and discovery. Such a shift in instructional methods is coincident with our objective of teaching for deeper understanding of quantum behavior with the expectation of later transfer of understanding. For this purpose we plan to:

(1) design activities and concept questions for students studying in groups in recitation or with trained peer leaders and, when this infeasible, for use in an interactive lecture format (Mazur, 1997);

(2) design these activities around investigations of computer simulations of quantum behavior;

(3) coordinate laboratory experiments with study group assignments and computer explorations.

Objective 4: ***Gather data on the effectiveness of our software and instructional methods for teaching students quantum concepts.*** In support of the above objectives, Professors Garik and Kelley, the project evaluator, with the assistance of a graduate student, will investigate carefully how students' conceptions of quantum behavior are built, how students transfer these concepts to other topics in chemistry, and what the impact is of the novel instructional formats. An outcome of this process will be a Quantum Concept Inventory, akin to the Force Concept Inventory of misconceptions in mechanics (Hestenes, Wells & Swackhamer, 1992). This will serve as a guide for instructors engaged in modern science and technology education to assess their students' backgrounds.

Objective 5: ***Design materials for national use.*** We will design our materials and methods with the input of instructors of general chemistry at other institutions. We are especially interested in involving community college faculty. Through workshops with consulting professors during the first and second summers, and responding to their needs, we will prepare for national dissemination.

Specifically to support this objective, we have designed our project to include (1) an Advisory Board of nationally recognized chemistry educators who are geographically distributed; and (2) enlisted the services of the New England Board of Higher Education to support our recruitment of instructors representing a spectrum of higher education institutions for our project.

Finally, we will design a survey to be distributed to general chemistry instructors nationwide. This survey will be aimed at polling the instructors' attitudes towards quantum concepts in general chemistry.

Objective 6: ***Design materials for web dissemination.*** To provide for the widest accessibility of our materials for both instructors and students, all materials will be designed for easy internet access and with the eventual goal of supporting distance learning. We will rely upon instructors/consultants invited to our summer workshops to provide us with feedback on the web presentation of our materials.

III. Project Significance

1. We are proposing to move the content and methods of instruction for general chemistry toward what the chemistry course of the year 2050 must look like by developing new methods of teaching quantum science concepts.
2. Our project instructional methods will be aimed at supporting in-depth inquiry by students enrolled in science courses of varying sizes, both large and small.
3. At the completion of the project we plan to have in place novel instructional materials and methods that can be used at other institutions. The instructional tools and supporting materials will be available over the web; the instructional methods will be disseminated through annual self-supporting workshops. The web site will be constructed to support and encourage use of our materials from a distance.

IV. Background

Software for a Descriptive Introduction to Electronic Structure

This proposal is based on our prior project Quantum Science Across Disciplines (QSAD) funded by the National Science Foundation (NSF REC-9554198; 5/1/96 -- 4/30/99; 5/1/99 -- 4/30/01 no-cost extension) to investigate methods for teaching quantum science to high school and undergraduate students using interactive graphical computer software. Professors Garik (PI) and Dill (co-PI) collaborated on this project. At Boston University Professor Dill piloted lecture presentations and selected software with his students in the context of general chemistry, and Professor Garik used the software in his integrated sciences course for pre-service elementary school teachers. In high schools we investigated how teachers taught with our materials and what their students learned.

The interactive Java software visualization tools we created bypass mathematical analysis to support real time interactivity with simulations designed for students to learn the basic concepts of energy levels, transitions between energy levels, the electron cloud model, the nature of molecular bonds, and the structure and charge distributions of important molecules. Multiple representations (2-d and 3-d) are offered to assist students' understanding of scale and structure. With these tools, quantum concepts and electronic behavior emerge in a descriptive language of shape, location, and color. Graphics are commercial quality. Examples are in the Appendix (also http://qsad.bu.edu). The QSAD Quantum Explorers (Atomic, Bond, Diatomic, Polyatomic, and Spectrum Explorers) are ready for use as a *component* of the proposed project. Currently the calculations are based on Extended Hückel molecular theory for computing molecular orbitals and Roothan-Hartree-Fock atomic orbitals for display purposes. These computations are fast and accurate enough to preserve the trends of the Periodic Table.

The Quantum Science Across Disciplines project was a proof of concept that software for teaching quantum concepts to novices can be created. However, the QSAD software by itself lacks the structured environment and detailed supporting materials necessary to make it usable by a wide audience of students and instructors. The project proposed here is to extend in an informed manner the QSAD software through the development of instructional material and techniques appropriate for undergraduate education. In this process, some of the existing QSAD software will need to be modified or significantly extended in order for the materials to serve the foundational role envisioned.

QSAD Lessons Relevant to this Proposal

1. We studied high school chemistry students in classes using the QSAD software, and compared them to students taught with a traditional approach. Concept maps were used to explore the students' understanding. For our assessment, special attention was paid to student explanations of the relationships among eight concepts: bonding, color, electronic structure, energy, molecular geometry, periodic trends, polarity and solubility. The control and experimental groups showed marked increase in forming propositions in five areas: bonding to electronic structure, electronic structure to periodic trends, molecular geometry to polarity, polarity to solubility, and color to energy. However, the experimental classes improved their ability to explain the relationship between five additional pairs of chemical concepts including: bonding to energy, bonding to polarity, bonding to molecular geometry, and polarity to molecular geometry and solubility (Hurwitz, Abegg, Garik & Nasr, 2000).

(2) We worked intensively with chemistry teachers (Robblee et al, 2000). We found that the greatest learning benefits occurred in classrooms where teachers fostered student inquiry using group investigations centered on the software. These teachers reported that their students offered new, more sophisticated explanations for single, double, and triple bonds after using the software; identified the cause of electronegativity in terms of energy levels and ionization energies as opposed to arguing teleologically that electronegativity arises from how close the atom is to having a complete valence shell; and, discussed how bonding orbitals shield nuclei from repelling each other, while antibonding orbitals expose nuclei to each other and so are less energetically favorable for binding a molecule. The explanations students offered can be accounted for by the visual images of atoms and molecules, which the software provides.

(3) We conducted in-depth pre- and post-interviews with high school students (Eshach & Garik, 2001, 2002a). These interviews provide us with insights necessary to assess baseline understanding and post-instruction learning for formative analysis of our proposed materials. From these interviews we constructed a detailed understanding of students' conceptual difficulties with quantum ideas. These range from their personal constructions of mental images intended to reconcile the model of the Bohr atom with an electron in orbit with the electron cloud model; to recurrent misconceptions held by students regarding the concepts of energy levels, unoccupied orbitals, and molecular bonds; and, deficits and misconceptions of prerequisite content such as Newton's Laws, electrostatic forces, and concepts of probability. We have further unpublished data from interviews with undergraduates.

(4) We conducted interviews with experts in order to learn how they (practicing chemists and physicists) think about quantum phenomena (Eshach & Garik, 2002b). The rich set of analogies and metaphors that we documented, and their use of multiple models, has enriched our perspective on how to design curriculum materials.

(5) We have assessed student understanding of quantum concepts, and related concepts, in the general chemistry course at Boston University. This past semester we administered pre- and post-questionnaires to all students taking the on-sequence general chemistry course for science concentrators. Students were queried on fundamental prerequisite concepts (wave, energy, and force concepts), information they may have brought from high school (meaning of quantum numbers; location of electron in hydrogen atom). The organization of the questionnaire was based on the work referred to above (Eshach & Garik, 2001), and instructors' input. Because of the multi-instructor format of the general chemistry course, the outcome of this learning assessment is mixed, and provides a baseline, not an evaluation of QSAD materials.

(6) Professors Dill and Garik have piloted the QSAD materials at Boston University. Prior to the QSAD project, Professor Dill developed lecture notes, required for the course, on quantum concepts for use with the general chemistry class (Dill, 1998). With the QSAD software, Professor Dill has extended the range of this quantum instruction. Each of the last two years, he taught the students in his lecture section (about 250) how to sketch wave functions manually for an arbitrary potential by identifying the kinetic energy with the wave function's curvature. Once students mastered the drawing of wave functions (which they did!), they used the Shooter, a QSAD applet designed by Prof. Dill, to solve the Schrödinger equation by varying the energy and observing whether the resulting curve matches the boundary conditions for the potential. This year Professor Hoffman and Mr. Crosby also used the Shooter for demonstration purposes in the honors chemistry course.

Professor Garik teaches an integrated sciences course for pre-service elementary school teachers. These students use the QSAD software to investigate the geometry of atomic orbitals, covalent and ionic bonding, and spectroscopic transitions. (Students in this class were appalled to learn that the Bohr model did not describe chemical behavior and demanded to know why so much of their high school instruction and their college text dwelled on this model.) Linked to these software activities are spectroscopy labs.

Related software materials**:** Software packages, like Spartan by Wavefunction, Inc., have been adapted for upper level college courses. The interfaces of these professional programs are not appropriate for introductory instruction. The NSF Visual Quantum Mechanics project at Kansas State University (Dean Zollman, PI) introduces physics students in college courses, and high school teachers and students, to quantum concepts. The project Practical Quantum Mechanics (E.F. Redish, PI, University of Maryland) is for engineering majors at the junior and senior level who have had a prior course in calculus-based physics. We have shared QSAD software with both groups. The difference between a physics and a general chemistry approach makes our efforts distinct. The Maryland group found the level of our materials inappropriate for upper division engineering students. Professor William Vining (University of Massachusetts, Amherst), who has had FIPSE and NSF support for his computer tutoring program for general chemistry, is interested in using our materials with his students (see letter of support).

V. Research Context

Research on Computer Modeling and Chemistry Instruction

Careful studies to determine if computer visualization and interactive software supports greater learning are difficult to conduct. However, recent studies support this contention. One of these used a computer program (Genscope) for instruction in genetics for high school students (Horwitz & Christie, 1999; Hickey et al, 1999). The fundamental finding is that if care is taken to provide the control and experimental classes with comparable assessments, students in the experimental group do learn more.

In another study with high school chemistry students, the researchers compared instruction between classes where interactive computer simulations and molecular modeling kits were employed with classes where neither of these materials were employed. The outcome was that the students who used the modeling materials (computer and physical) showed a significant narrowing of the gap between the lowest and highest performers on the pre-test at the time of the post-test. This narrowing of the performance gap was not observed for the control group. Students in the experimental group were also more likely to use graphical means to answer questions indicating a better understanding of molecular geometry (Dori and Barak, 2001).

At the college level, students' understanding of the particulate nature of matter, a well-recognized conceptual problem for chemistry students (Gabel, 1999), has been shown to improve after exposure to computer animations in lecture and/or access to such in a computer lab (Williamson & Abraham, 1995). The researchers distinguished between performance on exams where algorithmic problem solving obscured the demonstration of conceptual understanding, and performance on an instrument specifically designed to assess conceptual learning.

Theoretical Framework for the Proposed Project

In designing and evaluating our software and activities with students, we will rely on a constructivist approach. The vocabulary of conceptual change frames our work (Posner, Strike, Hewson & Gertzog, 1982; Hewson & Hewson, 1983). Before students can benefit from the computer software, the computer activity must be made *intelligible* through prior discussion and activities. The results of the computer software must further be shown to be *plausible* by relating them to experiment and by the interactive testing of the software results through guided exploration. Finally, the student must find quantum concepts to be *fruitful* by using the computer software to answer self-generated questions.

In our interviews with students, and in our analysis of their test responses, we will further look for changes in ontological perspective on the nature of the interaction between atoms that gives rise to molecules (Slotta and Chi, 1999). Students should not leave the chemistry course believing that chemical bonds are material substances (e.g., there are covalent, ionic, and polar covalent bonds, and perhaps that they are kind of stick-like). Such a view of bonding does not lend itself to conceptual transfer to other kinds of bonding (e.g., hydrogen bonding), or to predictions of the electronic properties of the solid state.

We agree with other authors that teaching concepts, as opposed to algorithms, is important to ensure students' capacity to think about chemistry (Gabel and Bunce, 1994; Gabel, 1999). Based on our work with high school students prior to their introduction to quantum concepts, we are expecting students to borrow from their classical science instruction a host of strategies to make sense of atomic level electronic behavior (Eshach & Garik, 2001). Some of this sense making will lead to misconceptions since quantum behavior is so different. We will study carefully the strategies necessary for students to arrive at an adequate conceptual understanding of the quantum nature of matter.

VI. Proposed Materials Development

Based on our pilot teaching, the course materials and manuals we plan to develop will combine:

- a description of mechanisms to re-utilize lecture time for experimental demonstrations, hands-on experiments by the students, and computer-based activities;
- creation of new laboratory activities and linkage of existing ones to the new topics;
- creation of software based activities with existing and extended QSAD software; and,
- homework assignments and study group activities based on Quantum Concepts software.

At the end of the project we will produce a text that will embody the pedagogical content knowledge we develop during the project, i.e., the knowledge of how to combine experiments, investigations, metaphors, and content knowledge to provide students with an in-depth appreciation of quantum concepts (Shulman, 1986).

The swiftness with which students obtain the latest computers is implicit in our assumptions about the materials we can develop. Group work in class, or in informal settings, is possible since so many students have laptop computers. Even at institutions with less advantaged students, the use of computer labs makes the materials we intend to develop accessible to all students.

Modules for Teaching Quantum Concepts

We will develop curriculum modules to be distributed over one semester of the general chemistry course and occupy roughly half the time. These modules will include:

Wave Exploration: The mystery of quantum behavior is in the wave-particle duality of matter.

What students will do: The vocabulary of wave behavior will be introduced to students through laboratory experiments (ripple tanks, standing waves in elastic media, optical interference and diffraction). Class discussion and demonstrations will focus on the nature of constructive and destructive interference, the spatial and temporal periodicity of waves, and the relationship of amplitude to intensity. In class and study groups, students will superimpose waves of differing phase, frequency, and amplitude using Excel. (This activity has already been piloted.) In study groups, and individually, students will investigate the properties of light and its interaction with matter using home-lab materials developed for the NSF Project LITE (PI: K. Brecher; co-PI: P.Garik; http://www.bu.edu/smec/lite).

Probability Exploration: This is a lead-in to an exploration of wave functions. The basics of probability, the analogy between probability amplitude/probability intensity and the amplitude of an electromagnetic wave and its intensity, the need for normalization, and the connection between wave functions and measurements, will be introduced to students.

What students will do: For this, we plan to add a tool to the Atomic and Diatomic Explorers that permits students to select volumes of space and determine the probability of finding an electron in this volume. Investigation of the interplay of low apparent density but large volumes farther from the nucleus will clarify the visual intensities. This activity can be done individually, or in discussion or study group.

Schrödinger Exploration: The association of a wave function with the discrete (quantum) energy levels observed in nature does not lend itself to classroom derivation. Students need an intelligible introduction to wave functions, one that provides a plausible link to experiment. Professor Dill has piloted this approach in CH102. Students are taught to draw wave functions based upon the proportionality of the curvature of the amplitude with the negative of the product of kinetic energy and amplitude. To master this approach students must be supported to understand kinetic and potential energy plots. By this means he has taught students to draw the wave functions for different families of potentials.

What students will do: For this exploration the manual activity is the drawing of wave functions; the subsequent computer activity is with the Shooter applet to find the energies of wave functions with a few loops for multiple square well potentials with varying barrier heights and spacing, a linear potential, and a harmonic potential. The study group leaders will lead discussions about the correspondence between large amplitudes for the wave function and the corresponding likelihood for locating the particle in a given region. Further discussion to interpret the double square well potential as the superposition of one square well wave functions will serve as a prelude to molecular bonding.

One Electron Exploration* – *What students will do: This activity is a direct outgrowth of our pilot study. In class, students manually sketch solutions for the five lowest energy solutions for a Coulombic potential. In the computer laboratory and at home, students then use the Shooter program to find the five lowest solutions and compare the solutions with their predictions. The Shooter also provides the energies for these states. For their laboratory activity, the students observe the emission spectrum of atomic hydrogen. In their study group, the students will be challenged to discover the correspondence between the observed frequencies and the differences between energy levels. The Hydrogen Spectrum Explorer (developed for QSAD) can be used by students to discover the nature of the Balmer and the Lyman series.

Two Electron Exploration: The distribution of electrons around an atom is choreographed by their Coulombic interactions and the Pauli Exclusion Principle. Without the latter there would be no significant differences between elements, no Periodic Table, and no chemistry as we know it. To explore the consequences of electron statistics, two electrons suffice.

What students will do: In their study groups, students will be asked to predict the electronic distribution and emission spectrum for helium based upon their understanding of the hydrogen atom. In class, the statistical consequences of having two kinds of indistinguishable particles will be discussed. With the Two Particle Explorer software (to be developed for this project), students will investigate the energy levels and spatial distributions of two charged particles (bosons or fermions) in an attractive Coulombic potential. In the laboratory, students will study the emission spectrum of helium. In the study group, students will compare the observed emission spectrum with the energy levels obtained from the Two Particle Explorer. The students will also be asked to reconcile their initial predictions for the electronic structure of helium with what they have discovered. The insights of this exploration for chemistry are the Pauli Exclusion Principle and Hund's Rules.

Atomic Structure Exploration (Periodicity, Aufbau, and Pauli Exclusion): The basic properties of the elements as summarized by the Periodic Table are a consequence of the quantized structure of the atom. Using the Atomic Explorer, students will study the structure of multi-electron atoms and relate the orbital filling process and Hund's Rules to their earlier Two Electron Exploration.

What students will do: In study and discussion groups, the recurrence of the filling of *s*, *p*, *d*, and *f* orbitals will be used to explain families of elements, and the variation of orbital size and geometry will be related to periodic properties. In the laboratory, and as part of a class demonstration, the spectra of the alkalis will be studied. In study groups, or home assignments, the students will analyze these spectra, and relate them to the Atomic Explorer, to investigate shielding.

Bond Exploration: The Bond Explorer provides a simple model for the genesis of molecular orbitals. With this software (already developed) a single electron is shared between two atoms. Each atom possesses one atomic orbital. The energy and symmetry of the orbital, and the distance between nuclei can be varied

What students will do: Individual activities and activities in study or discussion groups will focus on applying the wave-like character of the electronic distribution to understanding bond formation. By varying the relative energy of the two atomic orbitals, and by varying the separation of the two nuclei, the students will investigate the nature of the continuum of the molecular bond between covalent and ionic. Constructive and destructive interference, as well as orbital overlap, will be investigated graphically to understand the symmetries of molecular orbitals. The students will study electronegativity and dipole moment as a function of the energy difference between the orbitals of the two atoms.

Diatomic Exploration: The Diatomic Molecule Explorer combines two atoms (currently for atomic numbers up to Ar, but for this project through Kr) into a molecule or a fragment and provides a display of the molecular orbitals, total density, and dipole moment as a function of interatomic separation.

What students will do: Individually and in study or discussion groups, students will investigate the trends of bonding that can be made based on the Periodic Table. Ionization energy, and equivalently atomic radius, will be related to the concepts learned in the Bond Exploration to explain the variations in dipole moment for diatomic molecules. In the laboratory students will investigate the solubility of different species and relate this to polarity of the molecules.

Valence/Hybridization Exploration: These activities will be based on the Polyatomic Explorer which presents three-dimensional images of molecular structure and electronic distribution. The current Polyatomic application will need modification for this project.

What students will do: Activities for this exploration will focus on hybrid orbitals and VSEPR. Imagine the effect of bringing an H atom near a C atom – a pod of density will extrude between the atoms. Bring another H near the C – another pod will emerge. Continue this process and the pods will emerge with angles corresponding to the hybridization of the central atom, as well as the directions of approach. By minimizing the energy, and discovering the appropriate symmetry, C can be compared to N which in turn can be compared to P, and O compared to S. Students will study the different VSEPR geometries by viewing sets of molecules. For deeper understanding, students will predict the effect of substitutions (e.g., from SF_6 to SF_5Cl) and then investigate such molecules. The polarity of classes of molecules will be alternately investigated in the laboratory and with the computer,

Additional Explorations: We plan to develop an Organic Exploration, a Solid State Exploration, and a Spectrum Exploration. The first will be based on the Polyatomic Exploration and will have students investigate and contrast properties of different organic molecules based on attached functional groups. The Polyatomic Explorer currently displays the dipole moment, relative atomic charges of constituent atoms, and the electronic density of any or all orbitals. Students will make atomic substitutions and observe the effects. The Solid State Exploration will be designed to support material from the text *Teaching General Chemistry: A Materials Science Companion* (Ellis et al, 1993). This will require new programming. Finally, to the Spectrum Explorer we will add the ability to import experimental spectra, and generate spectra based on available electronic transitions for a specified molecule.

VII. Project Evaluation

For the purposes of project evaluation, the six objectives stated earlier must be rephrased to be testable. For example, Objective 1, to create an eight-week introduction to the quantum aspects of matter for general chemistry students, is testable if we recognize that the objective of such development work is to provide students with a better understanding of quantum concepts. Below we turn our project's objectives into a set of testable questions. With each question is provided a summary of how the evaluation will be performed. Some of the objectives overlap for purposes of data collection. The result is a reduction to five major evaluation questions.

Question 1: Do students have a better understanding of the concepts of the quantum model of atoms, molecules, and bonding as a result of participating in this project? What role, if any, do the Quantum Concepts materials play in the conceptual development shown by the students?

Subquestions	Data Collection	Respondents	Schedule
What do the students know?	Interview with concept mapping Course examinations.	students students	pre/post interviews faculty determined
When did they learn what they know?	Observation of students engaged in activities	NA	weekly observations
What was the role of the Quantum Concepts software?	Questionnaires Observation	students NA	pre/post questionnaires

Question 2: What are the skills and attitudes of the students and the professors at the various stages of participation in the project?

Subquestions	Data Collection	Respondents	Schedule
What are the skills/attitudes of the students?	Questionnaires Observation Questionnaire	students NA study groups	pre/post questions weekly pre/post
What are the skills/attitudes of the consulting professors?	Questionnaire	faculty	pre/post questions

Question 3: Is the software and web site accessible, understandable, and useful to introductory level college chemistry students?

Subquestions	**Data Collection**	**Respondents**	**Schedule**
Do the students use the programs?	Questionnaire	students	end of semester
Do the students find the programs useful?	Questionnaire	students faculty	end of semester
Do the students find the website useful?	Reviews provided by users	students faculty	twice each semester

Question 4: Are the study groups effective in developing and maintaining student learning and interest? Are the peer leaders effective in maintaining the groups?

Subquestions	**Data Collection**	**Respondents**	**Schedule**
Is peer leader training useful?	Questionnaire	leaders	end of semester
Do study groups contribute to learning?	Questionnaire	students	end of semester
Are leaders effective?	Questionnaire	students	end of semester

Question 5: Are the dissemination plans and activities effective?

Subquestions	**Data Collection**	**Respondents**	**Schedule**
Are the dissemination plans effective?	Questionnaire	consulting faculty	end of session
Are the dissemination activities effective?	Questionnaire	faculty	end of Year 3

Data collection will be an ongoing activity from the beginning of the project. Questionnaires will be developed for each of the groups involved -- students in the classes, study group leaders, and consulting faculty. The pre/post concept maps will use the methods and procedure developed by Novak *et al* (1984) and used to evaluate high school students' learning of quantum science concepts (Hurwitz *et al*, 2000). All observations and interviews will be conducted by researchers who thoroughly know quantum science principles. Whenever possible, questionnaires will be administered to a course the year prior to intervention provide a control to evaluate the Quantum Concepts materials. The multiple data sources will be used to triangulate the data and provide more reliability for the findings.

VIII. Project Personnel

The senior staff for the project are Professors Peter Garik (PD), Dan Dill (co-PI), Morton Hoffman (co-PI), Dr. Alexander Golger (co-PI), and Mr. Alan Crosby (co-PI). Professors Dill and Garik collaborated for five years on the QSAD project. Professors Dill and Hoffman have worked together for many years teaching general chemistry. Dr. Golger and Mr. Crosby work closely with Professors Dill and Hoffman as instructors for the laboratories for general chemistry. Finally, Mr. Crosby and Professors Dill, Garik, and Hoffman are working together on a “minigrant” ($5000) on molecular visualization.

The proposed project evaluator, Dr. Kelley (Professor Emeritus, University of Massachusetts – Lowell), taught chemistry for thirty-five years, and has a long history of working with chemistry teachers and developing curriculum. Dr. Kelley is a trained and practiced project evaluator. She brings to our project the content and curriculum background to advise us and professionally evaluate our progress.

For the graduate research assistant for this research project, we will draw on the many qualified doctoral students in the science education program at Boston University.

IX. Management and Development Work Plans

There are two principal development strands for this project. The Materials Development team will consist of Professors Dill, Garik, Hoffman, Dr. Golger, and Mr. Crosby. The Evaluation team will consist of Professors Kelley and Garik, and the graduate student. The Materials Development strand will have four interlocking components: development of syllabus and textual materials, development of software, development of laboratory experiments, and development of a web site to promote dissemination.

Each of the content experts will have input on every aspect of the materials development, and the Evaluation team will provide a running formative analysis for the materials developers. As PD, Professor Garik will collaborate on nearly all aspects of the research. He is both a content expert and a science education researcher. He will take principal responsibility to work with the programmer to ensure maintenance of the web site, the scientific accuracy of the software, and the intelligibility of the interface. Prof. Garik will work closely with Prof. Kelley and the graduate student on the formative analysis, and the preparation of research articles.

Professors Dill and Hoffman will provide input on the interface and content of the programs. A large portion of their time will be devoted to the design of activities, and the preparation of the text materials, which will evolve into a manual. Professor Golger and Mr. Crosby will focus on the development of the accompanying laboratory experiments and the text to accompany these activities.

***External Faculty Consultants**:* During the first two summers we will invite faculty from local institutions to a one-week workshop/consulting period. Prof. William Vining of University of Massachusetts at Amherst has expressed interest in working with us (see letter of support). He leads the instruction in general chemistry and is interested in using our materials with his 1000 student course. Prof. G. William Griffin of Bunker Hill Community College has also expressed interest (see letter), as have professors at other local four-year and community colleges.

Additional faculty consultants and collaborators will be recruited with the aid of the New England Board of Higher Education, a group with extensive contacts with regional educational institutions. (See letter of support.)

Advisory Board: The following people have agreed to be members to be members of an Advisory Board for our project: Professor Loretta Jones (Chemistry, University of Northern Colorado), Professor William Vining (see above), Professor Nathan Lewis (Chemistry, California Institute of Technology), Professor Yehudit Dori (Science Education, Technion – Haifa, Israel), and Dr. Haim Eshach (Medical Education, Technion – Haifa, Israel). For budgetary reasons, meetings with the Advisory Board members will be held virtually over the internet, or at national meetings that we jointly attend (ACS, NARST). Aside from advice, the Board offers an opportunity to have our work more widely disseminated.

Organization of Peer-Led Study Groups: Beginning fall 2001, with a grant from the Peer Leaders Team Learning program of the National Science Foundation and matching funds from Boston University, Professor Hoffman began organizing his general chemistry course for chemistry concentrators (CH111/112) around peer-led study groups. The students in this course are divided into study groups with six or eight members plus one peer leader. The peer leader is a student who has already taken the course, and received training from the project staff on content, software, and the techniques to lead a group through a learning activity. The study groups meet each week to respond to a learning activity.

The work proposed here plans to use these study groups as test beds for our computer activities. We will evaluate carefully how students in these groups use our materials by observation, interviews, and assessment on examinations. Piloting with these study groups will provide experience for the design of individual and small group activities for the larger science concentrators' general chemistry course.

Formative development of our materials will take place in two different general chemistry course environments at Boston University. CH111/112 is the two-semester sequence for chemistry concentrators at Boston University. A typical class has about seventy students. CH101/102 is the two-semester sequence for science concentrators. It is in CH102 that the quantum material is currently taught. For this class, we are planning to investigate mechanisms to create either formal or informal peer study groups. We will also adapt the activities developed for the student groups of CH112 as assignments for students in CH102 and for use in the discussion groups led by graduate teaching fellows.

What follows is a summary of planned products. The work plan for the project is detailed in Tables I, II, and III.

End of Year One Products

Materials Strand – Year One

- Draft of activities for introducing quantum concepts into the general chemistry curriculum. Distributed over a semester, this draft will cover four weeks.
- For the chemistry concentrators, a set of activities to be performed in study groups with peer leaders, as well as for individual exploration.
- For the science concentrators, a set of activities for individual exploration, for small group work during lecture, and for group work during discussion sections.
- An extended version of the Shooter application that supports student investigation into arrays of potentials and tunneling.
- An extended Spectrum Explorer application that allows students to investigate the emission and absorption spectra of square and harmonic potentials, as well as the current Coulomb potential case.

- Beta version of the Valence/Hybridization Explorer based on the Polyatomic Explorer.
- Spectroscopy, solubility and polarizability experiments coordinated with Quantum Explorers.

Evaluation Strand – Year One

- An interview protocol and questionnaire for pre- and post-intervention evaluation of general chemistry students' understanding of quantum concepts.
- Baseline data of general chemistry students' conceptions of quantum behavior.
- Baseline evaluation of student response to activities designed for study groups.
- A questionnaire for use in evaluating the teaching styles of faculty at other institutions.
- Draft questionnaire to determine general chemistry instructors' attitudes about quantum concepts.

End of Year Two Products

Materials Strand – Year Two

- Second draft of materials for teaching quantum behavior. Materials will cover modules for six to eight weeks of a semester.
- A revised, better documented, and extended set of activities for student groups.
- Beta versions of the Two-Electron Explorer and the Solid State Explorer.
- Beta version of the Organic Molecule Explorer based on the Polyatomic Explorer.
- All materials and software available for download from a web site to serve the collaborating instructors at their local institutions.
- Initiation of discussions with publishers for distribution of our text and software materials.
- Professors Hoffman and Garik will present at meetings of the American Chemical Society results of the newly developed materials.

Evaluation Strand – Year Two

- Qualitative assessment of student learning after the intervention of the new materials based on a comparison of the interviews during this year with the baseline interviews in Year One.
- Quantitative assessment of the effect of the new materials intervention on student understanding of quantum concepts based on a comparison of questionnaire responses in Years One and Two.

- Presentation of a research paper on the baseline understanding of undergraduate students of quantum phenomena at annual meeting of the National Association for Research in Science Teaching (NARST).
- Baseline data on local general chemistry instructors' instructional methods and teaching of quantum concepts.
- A record of the evaluation of the project's materials by the consulting instructors.
- First results of nationwide survey of general chemistry instructors' attitudes about quantum concepts.

End of Year Three Products

Materials Strand – Year Three

- Final edition of text materials intended to support instruction in quantum concepts.
- Final editions of all Quantum Concepts software and scripted activities.
- Completion of discussions with a publisher for distribution of our text and software materials.
- Completion of web site repository of all materials developed for the project. This web site will be maintained by the BU Science and Mathematics Education Center for a period of at least four years.
- Presentation of materials at American Chemical Society Meetings (national and local).
- Workshop for general chemistry instructors at Boston University or as a Chautauqua short course.

Evaluation Strand – Year Three

- Summative evaluation.
- Papers presented at NARST and AERA on student learning and the effect of different methods.
- Journal articles detailing the interview protocols, the test questions, and the results with students.
- Evaluation of the success of general chemistry instructors in using our materials.
- Evaluation of success of web site in supporting general chemistry instructors at other institutions.

X. Project Sustainability

Sustaining General Chemistry Instructor Workshops: For maintaining workshops, our strategy varies with time. At the outset, we will be seeking beta test sites and collaborating instructors to develop our material. The New England Board of Higher Education (NEBHE) will assist us in identifying such instructors. (See Appendix: NEBHE Letter of Support.) By Year Three of the project, we hope to be partnering with NEBHE to obtain funding for regional workshops with our developed materials to reach community college instructors and high school teachers. Independently of the success of the work with NEBHE, we expect that there will be sufficient interest in the chemistry education community to institutionalize our workshops through the Chautauqua workshop format. We will also explore the possibility of developing a web-based workshop for distance instruction in our methods and materials.

Sustaining Text and Software Materials: In addition to creating a web archive of all of our materials, we will seek a publisher to distribute our materials in text and CD formats.

Table I: Materials Strand Work Plan for 9/1/02 through 5/31/04

Task	Academic Year 02-03	Summer 03	Academic Year 03-04
Software	Polish Atomic, Bond, Diatomic and Polyatomic Explorers. Storyboards for Spectrum and Hybridization Explorers	Complete beta versions of Spectrum and Hybridization Explorers and modifications of earlier software	Use software with chemistry and science concentrators. Storyboard Two-Electron, Organic, and Solid State Explorers
Activities documentation	Develop text to accompany Atomic, Bond, and Diatomic Explorers	Finalize text materials for modules for four weeks of course	Use developed text in courses. Begin writing text for new Explorers.
Experiments	Plan experiments coordinated with above Explorers	Complete designing and implementing coordinated experiments	Use experiments with students. Plan for new Explorers.
Web Dissemination	Establish web site for serving up applications, applets, and text	Post activities and downloadable applications	Monitor web usage by students and faculty; provide assistance to consulting faculty
Workshops/ Dissemination	Recruit chemistry instructors from local institutions for summer consulting/workshop	Consultancy/workshop with faculty from local institutions.	Visit consulting faculty; observe courses and students; monitor progress by email. Present at regional and national ACS meetings.

Table II: Materials Strand Work Plan for 6/1/04 through 8/31/05

Task	Summer 04	Academic Year 04 – 05	Summer 05
Software	Complete beta version of Two-Electron, Organic, and Solid State Explorers	Use software for six to eight weeks in general chemistry for chemistry and science concentrators	Polish final components of all applications. Package for web and CD distribution.
Activities/Text	Complete draft text for new Explorer activities (activities for 4 weeks); polish earlier text based on prior semester feedback.	Use activities for six to eight weeks in general chemistry for chemistry and science concentrators	Complete course manual and accompanying software. Full description of all activities and methods for student engagement.
Experiments	Complete designing and implementing experiments coordinated with new Explorers	Use experiments in general chemistry for chemistry and science concentrators	Write-up lab manual to accompany software and course manual.
Web Dissemination	Update web site for downloads of new materials	Support Boston University general chemistry courses; support faculty and students at collaborating institutions.	Final hardening of web site to ensure long term access to all materials.
Workshops/ Dissemination	Second workshop for five consulting faculty; apply to host Chautauqua short course; seek academic publisher for text and software.	Visit consulting faculty; observe courses and students; monitor progress by email. Present at regional and national ACS meetings.	Submit manuals and software to academic publisher. Host Chautauqua short course, or host workshop for paying instructors.

Table III: Evaluation Strand Work Plan for 9/1/02 through 8/31/05

Task	Academic Year 02-03	Summer 03	Academic Year 03-04
Evaluation	Pre-test, post-test, and interviews for chemistry and science concentrators in general chemistry.	Analyze student data; design new tests based on data; interviews and questionnaire about teaching practices, for consulting faculty.	Pre- and post-tests for courses; monitor consulting faculty; prepare papers based on prior year's data.

Task	Summer 04	Academic Year 04 - 05	Summer 05
Evaluation	Analyze data from prior academic year; formative analysis feedback to Materials developers; prepare papers for NARST and AERA	Collect pre- and post-test data; interviews with students; track faculty at cooperating institutions; present at NARST and AERA.	Final formative analysis to inform end of project texts and web site. Final data analysis and completion of papers. Summative evaluation.