Proposed INTENSIVE FACULTY TRAINING WORKSHOP IN QUANTUM CHEMISTRY

Project Objectives

At the end of the workshop the trainees will be able to:

1. Relate the formalism of quantum mechanics to chemistry concepts and techniques such as the periodic table, electronegativity, bonding, aromaticity, color and spectroscopy.

2. Understand the mathematical methods used for developing models for chemical systems such as solving differential equations and use of matrix and vector methods.

3. Understand systems with exact solutions and why approximations are necessary for complex chemical systems such as multi-electron atoms and molecules

4. Understand the methods of approximation applied to complex systems such as perturbation method and the variational principle.

5. Understand the techniques of constructing the total wavefunction for complex systems and the use of symmetry.

6. Gain experience in solving problems covering theory and applications.

7. Gain experience in the use of internet based teaching resources.

Methodologies:

1. Lecturer and principal resource person will be Dr. Cynthia Juan Jameson, Professor Emerita, Univ. of Illinois , Chicago Circle. Dr. Jameson, besides doing outstanding research in nmr spectroscopy, has extensive experience in teaching undergraduate and graduate courses in quantum chemistry at the University of Illinois at Chicago (1968-2005) and in the University of the Philippines (1965-67). Her curriculum vita is attached.

2. The course will use Quantum Chemistry by Ira N. Levine (Prentice-Hall), 5th ed., or latest edition as textbook.

3. Dr. Jameson has proposed a two-week (12 days) schedule of lectures, discussions and supervised study group sessions. The proposed syllabus and calendar are shown below. The syllabus specifies the background knowledge which trainees must review before the course begins

4. Class will be divided into study groups of 4-5 students.

5. Lecturer provides one discussion period for every two lecture periods. Discussion period may be used for clarification, recapitulation, answering questions, showing additional examples and discussion of the solutions to the problem sets already completed by the trainees.

6. After each lecture, each study group of 4-5 students will write down the questions they have from the preceding lecture during a 10 minute caucus.

7. Study groups have two-hour periods in the afternoon, plus the after-dinner periods to: a) work on problem sets and b) resolve conceptual questions which arise from caucuses. At the end of the day, each study group discusses their remaining unresolved questions. This way, any ambiguities and misunderstood parts of the lecture can be cleared up before the next day starts.

8. Method of instruction requires a live-in type of accommodation for trainees and lecturer.

9. The URLs for supplementary web material and problems from the current literature will be provided.

10. At the end of the course, trainees will be given electronic copies of the lecture slides, the problem sets in a word-processing format, problem set solutions, supplementary materials with URLs for web sources, and a large number of sample examinations together with their detailed solutions.

Course Calendar

Lecture #	Topic	Readings Levine Qntm Chem	Problem Set
1,2	**Motivation:** Why do chemists need to know QM? **1. Introduction to Quantum Mechanics** Postulates of QM: definition of a wavefunction, operators, eigenvalues, eigenfunctions, Schrodinger Eqn	Chap 3, 1,7	1. Operators and acceptable functions
3	Example: Particle on a Ring		2. Eigenvalues, eigenfunctions
4	Example: Particle on a line	Chap 2	3. Separation of variables
5,6	Separability of a problem: Separation of variables		4. Expectation values
7,8	Expectation values	Chap 3	5. More separation of variables, Postulates 0-3
9	Building functions from a complete set	Chap 7	6. Superposition of states
10-11	More about operators: Hermitian, commuting operators		
12-13	Standard deviation of a series of measurements: The uncertainty principle		7. Uncertainty principle
14	Time-dependent Schrodinger Eqn stationary states, constants of the motion		
15-17	**2. Angular Momentum** Classical angular momentum→QM operators Eigenvalues and eigenfunctions of L_z Simultaneous eigenfunctions of L_z and L^2 Examples of particle on a sphere, the rigid rotor Raising and lowering operators	Chap 5	8. Angular Momentum
18-20	**3. An atomic orbital: solutions to the H atom** Separation of translation from internal motion Separation into R, Θ, Φ, Solution of the Φ part, m_ℓ The Θ part, ℓ, the relation between ℓ and m_ℓ The R part, n, the relation between n and ℓ	Chap 6	9. Hydrogen atom
21	**4. Matrix representation of QM** Operators and wavefunctions Eigenvalues and eigenvectors of matrices		
22	More angular momentum, the electron spin Matrix representation of angular momentum operators, NMR and EPR examples Coupling of spin and orbital angular momentum	Chap 10	10. NMR of nuclear spins

23	**5. Electronic structure of atoms** Many-electron atoms, statement of the difficulty Indistinguishability of electrons and of spins, Pauli exclusion principle	Chap 11	
24-25	The one-electron-at-a-time approximation for atoms, the Slater determinant as an expression of the Pauli exclusion principle in many-electron systems		
26-28	Electronic structure of atoms, shielding and effective nuclear charge, the Periodic Table, Electronic states of atoms, atomic spectra with spin-orbit coupling		11.&11A Atomic spectra, photoelectron spectra, properties of many-electron atoms
29	**6. Approximation methods** Perturbation method for non-degenerate systems	Chap 9	
30	Perturbation method for degenerate levels, example: crystal field theory		12. Applications of perturbation theory
31	Approximation methods: Variational method	Chap 8	
32	**7. Molecules** Separation of electronic and nuclear motion: the Born-Oppenheimer approximation		
33	A molecular orbital: the exact solution to the electronic motion in the H_2^+ molecule ion	Chap 13	
34	Characteristics of molecular orbitals: angular momentum, symmetry		13. MOs of diatomic molecules
35	Electronic states of diatomic molecules		
36	Solution of the nuclear motion problem in diatomic molecules, the angular part: rotational motion	Chap 4	
37	The radial part: vibrational motion		
38	Molecular states of a diatomic molecule, symmetry, including spin		
39	**8. Molecular Spectroscopy** Interaction between molecules & electromagnetic radiation		
40	Selection rules and transition moments, Lambert-Beer law		
41	Molecular energy levels and states		
42	Transitions between different electronic states		14. Examples of uV-vis absorption, fluorescence spectra of diatomics
43	Transitions within the same electronic state: Vibration-rotation spectroscopy		15. IR and microwave spectra of diatomics
44-45	Symmetry of states of polyatomic molecules, Vibration-rotation spectroscopy of polyatomic molecules	Chap 12	16. Spectra of polyatomics

12-day schedule

Typical daily schedule	Day 1	Day 2	Day 3	Day 4	Day 5	Day 6
8-8:50 **Lecture**	Lecture#1	Lecture#5	Lecture#9	Lecture#13	Lecture#17	Lecture#21
10 min caucus[a]						
9-9:50 **Lecture**	Lecture#2	Lecture#6	Lecture#10	Lecture#14	Lecture#18	Lecture#22
10 min caucus						
10-10:30 snack break/discussion[b]						
10:30-1:20 **Discussion**	Discuss#1,2	Discuss#5,6	Discuss#9,10	Discuss#13,14	Discuss#17,18	Discuss#21,22
10 min break						
11:30-12:20 **Lecture**	Lecture#3	Lecture#7	Lecture#11	Lecture#15	Lecture#19	Lecture#23
10 min caucus						
12:30-1:30 LUNCH						
1:30-2:30 **Study Group**[c]						
2:30-3:20 **Lecture**	Lecture#4	Lecture#8	Lecture#12	Lecture#16	Lecture#20	Lecture#24
10 min caucus						
3:30-4 snack break/discussion						
4-5 **Study Group**[c]						
5-5:50 **Discussion**	Discuss#3,4	Discuss#7,8	Discuss#11,12	Discuss#15,16	Discuss#19,20	Discuss#23,24
10 min break						
6-7 DINNER						
Study group[c] discuss unresolved questions from the day's caucuses and work on problem sets together.						

Lecturer provides one discussion period for every two lecture periods. Discussion period may be used for clarification, recapitulation, answering questions, showing additional examples.

[a]The 10 min caucus: After each lecture, each study group of 4-5 students will write down the questions they have from the preceding lecture (unknown terms, concept not understood, clarification required, etc.).

[b]Further discussion of what needs clarification takes place informally during the snack break, during which time mingling between study groups to exchange questions takes place.

[c]Study groups have two one-hour periods in the afternoon, plus the after-dinner period to (a) work on problem sets, (b) resolve conceptual questions which arise from caucuses. At the end of the day, each study group discusses their remaining unresolved questions. This way, any ambiguities and mis-understood parts of the lecture can be cleared up before the next day starts.

Trainees will need one ring binder with filler paper for lecture notes, another binder for problem sets, one spiral notebook per study group for writing questions arrived at in the caucuses.

Typical daily schedule	Day 7	Day 8	Day 9	Day 10	Day 11	Day 12
8-8:50 **Lecture**	Lecture#25	Lecture#29	Lecture#33	Lecture#37	Lecture#41	Lecture#45
10 min caucus[a]						
9-9:50 **Lecture**	Lecture#26	Lecture#30	Lecture#34	Lecture#38	Lecture#42	Lecture REV
10 min caucus						
10-10:30 snack break/discussion[b]						
10:30-1:20 **Discussion**	Discuss#25,26	Discuss#29,30	Discuss#33,34	Discuss#37,38	Discuss#41,42	Discuss#45
10 min break						
11:30-12:20 **Lecture**	Lecture#27	Lecture#31	Lecture#35	Lecture#39	Lecture#43	Discuss/Close
10 min caucus						
12:30-1:30 LUNCH						
1:30-2:30 **Study Group**[c]						
2:30-3:20 **Lecture**	Lecture#28	Lecture#32	Lecture#36	Lecture#40	Lecture#44	
10 min caucus						
3:30-4 snack break/discussion						
4-5 **Study Group**[c]						
5-5:50 **Discussion**	Discuss#27,28	Discuss#31,32	Discuss#35,36	Discuss#39,40	Discuss#43,44	
10 min break						
6-7 DINNER						
Study group[c] discuss unresolved questions from the day's caucuses and work on problem sets together.						

By the time the 12 days are over, the members of each study group will know each other so well that they are likely to provide support for each other when questions arise while they are lecturing physical chemistry.

WHAT YOU SHOULD KNOW OR REVIEW BEFORE WE BEGIN

Concepts from college physics which you are expected to know (review them):

- force
- velocity
- acceleration
- linear momentum
- angular momentum
- kinetic energy
- potential energy
- units of energy and conversions between them
- electrical charge
- electric field
- magnetic field
- electric dipole moment
- magnetic dipole moment
- behavior of charged particles in the presence of one another, a charged particle in an electric field, a charged particle in a magnetic field, an electric dipole moment in an electric field, a magnetic dipole moment in a magnetic field

Elementary mathematical concepts and operations which you are expected to know (review them):

- derivative
- integral
- complex numbers
- simple differentiation
- partial differentiation
- integration
- trigonometric relations
- solution of a quadratic equation
- vectors in 3-dimensional space
- solutions of simultaneous linear equations in x, y, z
- standard deviation

Reading material print and web:

Ira N. Levine, Quantum Chemistry 5^{th} edition paperback is a good first resource for the course.
URLs for supplementary Web material will be provided
Problems based on current scientific literature will also be provided.