Philosophy behind the plan for the intensive course in Quantum Chemistry

Cynthia J. Jameson, University of Illinois at Chicago

1. Emphasize deep understanding of basic concepts, not so much the mathematics. The goal is that trainees come away from the course with a firm foundation on which to build. I won't show them everything, but I expect that what they will see they will understand well enough so as not to be confused when they are teaching the subject. Towards the goal of deep understanding, trainees of the workshop need to be provided with many opportunities to ask questions to clear up misconceptions or get explanations for nagging doubts, as early as possible.

2. Provide sample problems which bring quantum mechanics (QM) to bear on related chemistry concepts: the periodic table, electronegativity, bonding, aromaticity, color, spectroscopy, so that QM is not an isolated subject but the underlying theory which is necessary to understand all of chemistry. Chemical change and chemical structure involve electrons; that is why we have to think about these chemical concepts in terms of QM theory.

3. Provide examples which involve finite basis sets so that trainees see complete, exactly solvable problems in QM and do not equate QM theory necessarily with approximations such as those which arise from use of truncated basis sets. I use Nuclear Magnetic Resonance for this because nuclear spin angular momentum for ground state nuclei has a finite basis set of functions; besides, this example gives them a connection to a very useful spectroscopy.

4. Introduce perturbation theory, matrices, variational methods, symmetry which are powerful ways of thinking about systems and properties, applicable to a wide variety of applications. I will use some chemical applications of these concepts in lectures or problem sets so that trainees appreciate their power.

5. Provide a clear rendering of the one-electron-at-a-time (orbital) approximation. Chemists need a firm grasp of the one-electron approximation, which they instinctively use but do not really understand its ramifications. I will make clear why one-electron (i.e., orbital) methods fail, when deviations from this model are important, how large are such deviations?

6. Use spectroscopy as the primary experimental manifestation of QM so that quantum mechanical principles become clear.

7. Relate to partition functions, transition states, ensemble properties from single-particle properties.

8. Show trainees strategies for solving problems, not how to do math but rather how to think about the problem so that the postulates of QM can be applied. Necessary math background will be reviewed, as needed, where needed. As a starting point they need at least to have familiarity with differential and integral calculus.

9. Compensate for the fast pace by providing extensive access to the lecturer beyond lecture hours, i.e., discussion periods after every 2 lectures, plus problem-solving sessions. Ideally the content of this course (45 lecture hours) is spread out over one semester, but we will attempt total immersion of 8-plus hour days with lunch breaks, with intensive open discussions and small group sessions. Also we will attempt to sequester the trainees so as to completely focus on the workshop.

10. Split up the class into study groups of 4-5 each. Usually many students are missing the same points in lecture, but do not realize that others are in the same boat, and sometimes have difficulty figuring out what it is that they do not understand. Study groups' main purpose is for each trainee to discover what it is they do not understand during the 5-minute caucus after each lecture hour. This way they can decide what questions to ask the lecturer. Study groups will also work on problem sets together. The small group effort takes the place of individual effort on doing problem sets (with such a fast pace, the latter is not practical, some students will get left behind when they get stuck on how to start a problem). I will be available for the problem-solving sessions, of course, just that I will be seeing each group only a fraction of the time. The small groups will be constituted of trainees from different universities so that each individual can have 3 or 4 persons outside their own institution that he/she has worked very closely with, and who can provide help and moral support while teaching quantum chemistry.

11. Provide problem sets which are not merely exercises, and which make connections with the chemistry they already know and teach in lower level undergraduate classes. At the same time, I do not envision the participants doing a lot of number crunching because I would like to emphasize the understanding of the principles.

12. I will not follow a textbook but each trainee should have their own copy of Levine's Intro to QM.

LOGISTICS

1. Ideally, we will have the dormitories, dining room, lecture room and problem session rooms in the same building. I suggest that I live in the same general quarters as the trainees so they can talk to me outside of class, and have little or no travel time between classroom and accommodations. Also, ideally, the meals will be catered or ordered take-out so that all participants start and finish meals at the same time, such that 1 hour is adequate for lunch, similarly for dinner. The idea is that not too much time will be spent going back and forth; if transportation is required, much time is wasted in traffic and we also have to think in terms of having to make too many separate fail-safe arrangements (not so easy to do!).

2. Because of the nature of the course, each lecture is a prerequisite for the next; it is absolutely necessary for everyone to be present from the beginning. The fast pace makes it difficult for a latecomer to catch up. Ideally, all trainees check into the

dormitories the night before and the group stays together all 12 days. Nobody spends days or nights “off-campus” except for the middle Sunday which everyone is expected to spend entirely on R & R.

3. I think I will probably use a combination of overhead projector (using prepared transparencies) together with blackboard/whiteboard (big pad on easel will do, if there are no boards) as my primary lecture mode. I will also need during the discussion periods to be able to project from my laptop or the lecture room computer the pdf solutions to the problem sets they have already completed. It will be necessary for me to be able to give PowerPoint presentation on some parts of my lectures, and overhead transparencies on other parts, and have blackboard/whiteboard writing at the same time.

4. The space for the evening problem solving sessions could be the same as used during the day, or else we can use the dining room. We'll take whatever is practical. If dorm space is available for study groups, it will probably work even better.

5. The study groups do not necessarily have to have different rooms to work in, just enough space apart so that each group is truly independent of the others and can work without being disturbed by what is going on with the other groups, also, so I can talk to each study group separately without disturbing the others.

6. If any Ph.D. students also wish to take the course, giving them University of the Philippines graduate course credit would be very appropriate. The lecture schedule includes an entire semester's worth of lecture time and material. These participants will have the advantage that they will have the extra discussion period which I will give for every two lectures, plus the problem-solving sessions in groups of 4-5.

7. Any journal articles that can be used for making up examples and designing problem sets or exams I will collect here before I go because UP may not have the subscriptions to the electronic versions of journals. I will put all supplementary material into a CD that we can duplicate for the participants on site. That way each participant will have a collection from which he can pick out spectra, potential energy diagrams, tables, etc. for making up lecture examples or problem sets when teaching their course.

8. There is only one type of computer program I can think of that might be particularly useful for two problem sets I have. One is an angular momentum problem set, where I lead them through calculating an NMR spectrum of three inequivalent protons. Here they will need to be able to diagonalize a matrix and find its eigenvalues and eigenvectors. It is a very concrete example. For this they will need something like Mathematica, MATLAB, Maple or any other available user-friendly software that is already used there. I can bring my Mathematica. It would help if my graduate assistant(s) are very familiar with the software the trainees will use.

Optional:

Often there are good examples (animated graphics, etc.) in web sites that would be useful for them to know about so they can use those as illustrations when they are teaching. For this purpose we will need access to computers with internet connection for each study group of 4-5 students. Have at least 1-2 extra, just in case there are unexpected problems with the PCs. That way each study group has access and they can copy the url's into a document that they can e-mail to themselves when the course is over. They can do the same with downloads. It would be nice to have a collection of books and hand-outs for supplementary reading/browsing to be kept in a room where trainees have 24-hour access.

The venue for the Intensive Faculty Training Workshop on Quantum Chemistry: Bonifacio Hall of the School of Labor and Industrial Relations (SOLAIR), Jacinto St., University of the Philippines, Diliman, Q. C. The rooms set aside for the participants are labeled in yellow: