**COURSE SYLLABUS Spring 2016**

**CHEM 6854 Physical Chemistry**

**PROFESSOR:** Dr. Jerry Fong (Physical and Health Sciences Bldg room 305. Phone:#: 587-3692 . Campus e-mail: FONGJD)

**LECTURES: MWF 11**

**LAB: Wednesday 2-5**

**REQUIRED TEXT:** D. A. McQuarrie and J. D. Simon, **Physical Chemistry: A Molecular Approach**,

University Science Books 1997

**GRADING:** **Activity pts each # total % of Grade**

Exams 100 3 300 26.0

Homework 40 10 400 34.6

~Labs 40 13 4801 41.6

Final2 75 6.8

**Total 1155 100**

1 Lowset lab is dropped  2Final will consist of a 75 point oral examination

A: 90-100% B: 80-89 % C: 70-79 % D: 60-69% F: <60%

**Student Learning Outcomes:**

At the end of the course, successful students should be able to:

1. Recount and explain the major dilemmas in classical physics that led to the development of quantum mechanics : black body problem ,

photoelectric effect, discrete spectrum of H.

1. Describe and recount the 5 quantum postulates and how they are used to transform classical descriptions into quantum descriptions of motion.
2. Analyze and compute the eigen energies Ei , <pi > , <xi > for several 1D quantum mechanical systems including particle-in-a-box, harmonic oscillator and 2-body rigid rotor.
3. Construct from basic quantum rules, both the overall eigenvalue problem describing the H atom, as well as formulating the details of the analysis leading to the final solution of the H-atom, including series solutions of Laguerre and Legendre differentials.
4. Apply both perturbation and variational methods to the solution of the harmonic oscillator problem for diatomics, and for multi-electronic systems (e.g He, Li…) and from this analysis, derive critical spectroscopic constants (k, D, α for vibration; Ei and Hij overlap for electronic systems.)
5. Construct the energy manifolds and related optimized structures of molecules, intermediates and transition states using Spartan ChemQ software
6. Recapitulate and explain the four laws of classical thermodynamics.
7. Derive from the above four laws, expressions of ΔH, Cp and Cv and connections between ΔH and Cv, Cp and apply the latter to computations of gas behavior, bond energies, reaction heats and phase change energies
8. Derive from the above four laws, expressions of ΔG, ΔA and their connection to K

**Some Comments and Perspective on the Course and Material**

Of all the courses in a chemistry curriculum, physical chemistry easily ranks as the most feared and reviled. The subject bristles with highly technical language, forbiddingly abstract concepts and unrepentantly mathematical reasoning which, truth be told, are rarely used in most day-to-day applications of chemistry. Nonetheless, taking this course is a required `rite of passage’ for all card-carrying members of the chemical fraternity. Why?

It may be that it is simply the draconian hand of old school chemical pedagogy that forces us to. In that universe, the tradition of ***`no pain, no gain’*** (=curriculum rigor***)*** rules, and so does the “***if I had to take the &\*(^% course , you do too…***” (=curriculum depth and breadth).

My raison d’être for both teaching this course and believing in the requirement is quite different and frankly personal.

The body of knowledge spanned by physical chemistry represents irreducible principles upon which all chemical practice rests. Look for the reason we use hybridization models in organic chemistry and you will soon confront the quantum variational principle. Probe into what really underlies an IR spectrum and the Legendre harmonic oscillator solution materializes. Even when you want to understand something as `simple’ as the exchange of heat and work between a piston filled with an ideal gas and its surroundings, you end up neck deep in a consideration of q,w, ΔS,ΔHp, Cp and the 4 laws of thermodynamics. Bluntly, physical chemistry is the critical foundation you need if you really, really want to completely understand at the deepest level what’s going on in any chemical event.

It is also a highly disciplined mindset. The overarching approach in physical chemical reasoning is to focus on a small set of very simple physical models of chemical interest and **quantitatively** work out their behavior according the rules of physics with the help of appropriate mathematical tools and techniques. The numerical results of the simple models are then systematically and quantitatively compared against experimental results from real molecular systems and the deviations addressed with appropriate and sensible corrections to the original model assumptions. Once these are worked out to sufficient precision, more complex physical systems are described using the simple systems as the `basis set’ or, more picturesquely, as the Lego blocks for building something bigger and grander.

The game is ruthlessly rational, and potent. In the early 1980s, quantum calculations of the energy levels and structures of even small molecules were difficult and required the services of a university’s best main frame computers to produce poor-to-fair predictions. Now, you can buy a commercial `molecular quantum mechanics’ program for your lap top that not only reproduces exactly, the bond lengths and angles of most small to medium sized molecules, but which make respectable estimates of what an activated complex looks like during a specified reaction, and predicts the NMR, UV-VIS and IR spectra for both ground and excited state molecules that haven’t even been made yet. That’s some impressive cooking starting from the humble harmonic oscillator and 1D particle in a box.

Learning this material is also, for the instructor’s money, a rare chance for intellectual odyssey. His own journey as a young student attempting to master it whole was life-changing. If you’re game, really exploring physical chemical reasoning produces a deep delight, and an undeniable sense of accomplishment that only those who have really experienced it can savor. It can also be a humiliating, fear-soaked experience for those students who survive by just `passing the tests’ and who focus on grades, not understanding. That dog won’t hunt here. There is no substitute for honestly hiking through long hours reading and re-reading and re-re-reading pertinent sections of the text and gasping uphill to reach even a partial understanding of what’s been written. Nor is there any way you can test your paltry understanding except through climbing over many –often difficult-problems, and by surmounting your lack of understanding by asking questions both in class and out of both instructor and fellow students. This is one course where really understanding what’s going on and why is the only route home. It is not-to be frank- an easy trip. Do it in earnest, however, and it is the instructor’s promise he’ll guide you `upriver’ ,set you ashore, home free, with something, finally, to write home about.

**COURSE SYLLABUS : Chemistry 6854 (Physical Chemistry)**

**Week Dates Topics Covered (subject to change) Reading (McQuarrie text)**

**1 1/20-1/24 -Blackbody radiation; photoelectric effect, H-atom 1-25**

**-Bohr’s derivation of the H-atom’s electron energies**

**Heisenburg uncertainty in several forms**

**2 1/27-1/31 -Classical 1D Wave equation: basic physics 39-54**

**-Solving the 1D equations for various conditions**

**-extensions to 2D**

**3 2/3-2/7 -Schrödinger’s equation and 1D particle in a box 73-90**

**-ψ and <ψ|Â|ψ>**

**-quantum calculations for En, <p>, <x>, σ**

**4 2/10-2/14 -Particle-in a box (continued)**

**-Vectors ( a brief review) 105-112**

**-The 5 Quantum Postulates & the role of commutivity 115-133**

**5 2/17-2/21 -Applying the postulates to two classical systems**

**1) harmonic oscillator 157-173**

**2) rigid rotor 173-179**

***6 2/21 Take home exam 1 distributed due Monday 3/3***

**6-7 2/24-3/7 -Spherical Coordinates 147-153**

**- The H atom solved using Schrödinger’s equation 191-219**

**\*set-up in spherical form**

**\*separation of variables**

**\*the 3 associated Diff. Eq and their solution**

**\*typical calculations and plots**

**8 3/10-3/14 -Determinants 231-238**

**-Approximate methods 241-260**

**\*variational method**

**\*perturbation method**

**9 3/15-3/23 SPRING BREAK**

**10 3/24-3/28 Helium via perturbation pp 260; problem 7.30**

**H2+: introduction to molecular orbital methods 323-335**

***10 3/28 Exam 2-in class. Take home exam 2 distributed. Due Monday 4/7***

**11 3/30-4/4 Survey of Modern Quantum Molecular methods pp 411-433**

***12 4/7 Take home exam 2 Due***

**12-13 4/7-4/18 First Law of Thermodynamics 765-779; 780-800**

**14-15 4/21-5/2 Second Law of Thermodynamics and Entropy 817-844**

**16 ` 5/5-5/9 Free Energy Functions and their applications 881-887; 901-905**

**16 5/5 In-Class Exam III. Take home exam 3 distributed. Due day of Official P. Chem Final**

**17 5/12-5/16 *Takehome exam 3 due* . Final oral exam (time and date of Official P. Chem Final)**