ChE626A: Practical Introduction to Quantum Mechanical Methods for Scientists and Engineers (3-0-0-9)

Lecturer: Professor Vishal Agarwal
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Lectures: Monday and Wednesday, FB470, 5:10pm-6:25pm, **Be on time.**
Office Hours: _____ or by appointment

Assessment: 15% for Project 1 and 15% for Project 2, 35% for mid-sem, 35% for end-sem. **Zero-tolerance policy on academic dishonesty.**

Assignments: Reading and Home assignments.

Examination: 3hrs (both mid-sem and end-sem). One make-up exam at the end of the semester for those who missed the end/mid-sem with a valid reason.

Lecture-wise Breakup:

Topics	**Lectures**[a]
Summary of classical mechanics: conservation laws, Hamiltonian and Lagrangian formulation; The need for quantum mechanics;	1
Basic concepts: physical observables and operators, expectation values, Heisenberg's uncertainty principle, Schrödinger's equation	5
The many-body Hamiltonian, Born-Oppenheimer approximation, variational principle, the concept of potential energy surface; What makes electronic structure difficult	2
Hartree-Fock (HF) approach: restricted and unrestricted method, and their comparison with experiments	6
Localized and plane-wave basis sets; Pseudopotentials; Practical considerations such as choosing a basis-set	2
Self-consistent field calculations and Hartree-Fock code in Matlab[b]	1
Exercises with open-source quantum-mechanical package	2
Density functional theory (DFT): Hohenberg-Kohn theorems, Kohn-Sham formulation; Exchange and correlations: LDA and GGA approximations	6
Pure and hybrid DFT functionals	2
Tricks for self-consistent solution of the Kohn-Sham system: mixing and diagonalization techniques	2
Failures and successes of DFT: vander Waal's correction and DFT+U approach	2
Configuration interaction and Møller-Plesset perturbation theory	4
Applications of quantum-mechanical methods in engineering and sciences	2
Density functional theory code in Matlab	1
Exercises with open-source quantum-mechanical package	2
Specialized topics (if time permits): Ab initio molecular dynamics (Born-Oppenheimer and Car-Parrinello), ring-polymer molecular dynamics.	
Total	**40**

[a] Each lecture is of 50 mins duration
[b] Extra lectures for students unfamiliar with Matlab

Practice: In addition to theory lectures, there will also be two computer-related exercises in this course: a) Students will develop a HF and DFT code from scratch using Matlab. b) A few lectures will be designated as an exercise for performing calculations on an open-source quantum-mechanical code which will be used in homework assignments.

Teaching Assistants: Dewansh (dewanshr@iitk.ac.in)
Prosun Halder (halderp@iitk.ac.in)

Useful Text Books: Although there are several excellent books covering quantum mechanical methods, unfortunately there is no single book which covers all the topics mentioned in this course. The contents of this course will be drawn from several texts and research papers. Some of the texts which will be used are:

- **Text Books on Quantum Mechanical Methods**
  - "*Density-functional theory of atoms and molecules*", by Robert Parr and Weitao Yang, Oxford University Press, ISBN-10: 0195092767.
  - "*Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory*", by Attila Szabo and Neil S. Ostlund, Dover Publications, ISBN-10: 0486691861.
  - "*Molecular Electronic-Structure Theory*", by Trygve Helgaker, Poul Jorgensen, and Jeppe Olsen, Wiley-Blackwell, ISBN-10: 1118531477.
- **Text Books on Basic Quantum Mechanics**
  - "*Principles of Quantum Mechanics*", by R. Shankar, Springer, 2nd Edition, ISBN-10: 8181286863.
  - "*Quantum Mechanics*", by Claude Cohen-Tannoudji, Bernard Diu and Frank Laloe, Wiley VCH, Vol. 1, ISBN-10: 0471569526.
  - "*Quantum Chemistry*", by Ira N. Levine, Pearson Education India, 7th Edition, ISBN-10: 9332558531.
- **Other References**
  - "*Density Functional Theory: A Practical Introduction*", by David Sholl and Janice A. Steckel, Wiley-Blackwell, ISBN-10: 0470373172.
  - "*Introduction to Computational Chemistry*", by Frank Jensen, Wiley-Blackwell, ISBN-10: 0470011874.

Some Points to Keep in Mind.

1. **Learning is your responsibility.** This is a graduate level course and you must take responsibility to deeply understand the subject. Pay utmost attention during lectures, and keep up with the reading materials. Don't be shy, ask questions during lectures or after lectures. Please remember engaging is the best way to learn.
2. **Homework Problems.** First try working the homework problems independently. If you have difficulty moving forward even after several tries, please ask for help either from me during office hours or from TA's or from your peers. I encourage you to discuss homework problems in groups but when you sit down to finally write your homework, it should be done independently; and it should reflect your understanding of the problem.
3. **Grade is Just a Number.** Don't get into the race of just getting grades. Your aim should be to learn, understand, and master the subject. This requires a painful struggle through lectures, texts, and homeworks. Everyone has different backgrounds and has different speeds of learning; so invest the required time. Remember that: "Rome was not built in a day".
4. **Think Critically and Challenge Yourself.** Critical thinking is possibly one of the most important skill that will help you in whatever you do in life. This course is an opportunity to develop that habit. Think critically about what you read and about homework problems. Don't be satisfied by just solving problems or understanding course contents. Challenge yourself to go beyond the class lectures and homework problems.

Academic Dishonesty.

Please read the following carefully (taken from https://www.winona.edu/business/96.asp):

1. **Cheating:** Using or attempting to use unauthorized materials in any academic exercise or having someone else do work for you. Examples of cheating include looking at another student's paper during a test, bringing a crib sheet to a test, obtaining a copy of a test prior to the test date or submitting homework borrowed from another student.
2. **Deception and Misrepresentation:** Lying about or misrepresenting your work, academic records, or credentials. Examples of deception and misrepresentation include forging signatures, falsifying application credentials and misrepresenting group participation.
3. **Enabling Academic Dishonesty:** Helping someone else to commit an act of academic dishonesty. This would include giving someone else an academic assignment with the intent of allowing that person to copy it or allowing someone else to cheat from your test paper.
4. **Fabrication:** Refers to inventing or falsifying information. Examples of fabrication include drylabbing (inventing data) or making references to sources you did not use in academic assignments.
5. **Plagiarism:** Using the words or ideas of another writer without proper acknowledgement, so that they seem as if they are your own. Plagiarism includes behaviour such as copying someone else's work word for word, rewriting someone else's work with only minor word changes and/or summarizing someone else's work without acknowledging the source.

Pledge

I, do solemnly promise that

1. I will maintain the highest standards of academic honesty during this course.
2. I have carefully read above forms of academic dishonesty and I will not indulge in any of them. If I am caught indulging in any one of them, I deserve one and only one grade, i.e., **F**.
3. I will maintain at least 90% of attendance in this course.
4. I will not be late for this class.

***"Try not be a man of SUCCESS but rather try to become a man of VALUE"* — Albert Einstein**