Chemical Binding (CHM 621)

Instructor : K. Srihari office : FB 435 ✆ : 7043 email : srihari@iitk.ac.in

1 Course outline

The numbers in the □ indicate, approximately, the number of lectures to be given on that particular topic.

- H atom revisited and H_2^+ in the first pass. [3]
- Many electron atoms - perturbation, variations, and other approximations. Spin, term symbols, and wavefunctions. [10]
- Molecules - diatomic and polyatomics in the MO framework. Approximations. Valence Bond? [10]
- Modern electronic structure theory - many electron wavefunctions and operators, Hartree-Fock-Roothaan equations and basis sets. Sprinkles: DFT, Atoms-in-Molecule, what next? [19]

In this course you will be introduced to the quantum theory of molecular structure. In order to do this it is required to understand *multielectron atoms* first. Approximate but useful techniques like *variational* and *perturbative* methods will be introduced while we address the atoms. Later, the same approximations in slightly different avatars will be very useful when we discuss molecular structure. Important approximations like Born-Oppenheimer and *Hartree-Fock* will be used but not derived in the first half of this course. After getting an idea of the *Molecular Orbital* descriptions of bonding in molecules a brief introduction will be provided to various approximate theories. Notable among them is the *Hückel* approximation for π electrons. The remaining lectures will correct partially for the earlier handwavings and qualitative ideas by an explicit introduction to *modern* electronic structure theory. Note the word introduction in the previous sentence - we will barely scratch the surface of this vast field!

What you will not learn in this course is a fairly long list by itself. Topics like *coupled-cluster* methods, *configuration interactions*, the so called *complete active space* (CAS) SCF and *multireference* (MR) CI methods are a few in that list. An elective level course (unfortunately none exists as of now!) would quench your thirst in case you are thirsting for some more! Another important omission is that we will not talk about *Density functional theory*. Given the emerging importance of DFT it is rather unfortunate but that is all the time we have got and again a elective level course (perhaps titled "Binding chemical binding") would do justice.

2 ✓ Grading policy ✗

There will be regular homeworks in this course (approximately one every two weeks). Three exams (first and second midterms and the final) will be provided for advancement of your knowledge. First exam will be a in class open book/notes exam, the second will be a take home exam and the final will be in class closed book/notes exam. The homeworks will account for 25%, the midterms 25% each and the final will be worth 30% of the final grade.

3 References

We will be mainly following two textbooks

- ❏ D. A. McQuarrie and J. D. Simon, *Physical chemistry - a molecular approach*, Viva Low-Priced student edition, New Delhi, 1999. Chapters 8, 9, 10, 11. This book will be followed for the first three topics listed above.

- ❏ A. Szabo and N. S. Ostlund, *Modern quantum chemistry*, Dover reprint edition, NY, 1996. This book will be followed to some extent for the last part of the course.

There are many other books in our library which you can refer to. Some of them are listed below.

- R. S. Berry, S. A. Rice and J. Ross, *Physical chemistry*, Oxford University Press, 2000. This one is at an advanced undergraduate level. Chapters of relevance are 6,7,8.

- L. Pauling and E. B. Wilson, *Introduction to quantum mechanics*, McGraw Hill, 1935. This is a classic and I quote from the preface - "*In writing this book we have attempted to produce a textbook of practical quantum mechanics for the chemist...*". Later they go on to say (in 1935!) that "*...particularly designed for study by men without extensive previous experience with advanced mathematics, such as chemists..*". Chapters of relevance are VI, VII, IX, XII, XIII.

- Ira N. Levine, *Quantum chemistry*, 4th ed. 1991. This is a nice book and library has many copies. There are many interesting problems at the end of each chapter.

- J. A. Pople and D. L. Beveridge, *Approximate molecular orbital theory*, McGraw Hill, 1970. This is still a good book to refer to in the context of approximate methods and their utility in chemistry.

3.1 Websites of interest

You might find the following websites useful during the course.

① `www.hec.utah.edu/TheoryPage/`

This one is a introductory online course on Theoretical Chemistry by Jack Simons. Worth browsing through.

② `zopyros.ccqc.uga.edu/lec_top/lectures.html`

This is the Fritz Schaeffer page and contains advanced materials related to our course. Some of the things like coupled-cluster methods and details on configuration interactions will not be covered by CHM 621. If you are interested in these tpoics and other details you should get into this site.

③ `www.csc.fi/lul/chem/graphics.html`

This is a nice site for graphics and visualizations. It is quite extensive and links to other visualization sites over the world. You will find some interesting pictures of molecules (all kinds), animations of reactions and other fun stuff.

④ `web.lemoyne.edu/ giunta/papers.html`

Looking for classics..then some of them can be found here.

⑤ `www.quantum-chemistry-history.com`

History is important..it can give you a sense of belonging..

4 Note ✍

Submission dates of homeworks and the take home exam are not negotiable. Homework has to be submitted on acceptable quality paper!

5 Get to know them!