

# Physical Chemistry I (CHM 421)

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## 1 Outline

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

- ⇒ **Brief introduction to classical mechanics:** Lagrangian, Hamiltonian, and the variational formulation □4
- ⇒ **Principles of quantum mechanics:** History, wavefunction, interpretation, alternative formulations □6
- ⇒ **Quantization:** harmonic oscillator, plane rotor, angular momentum, tunneling, and simple exactly solvable models □10
- ⇒ **Atoms:** Hydrogen, introduction to many electron atoms □5
- ⇒ **Approximation methods:** perturbation theory, variational approach □10
- ⇒ **Applications:** Spectroscopy, bonding □10

In this course you will learn the basic principles of quantum mechanics. There is a rich history of this subject and our library has many good books that you can consult in this regard. Note that the principles of quantum mechanics are the same regardless of whether it is being taught in a chemistry, physics, or mathematics course - only the style and emphasis are different.

## 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 20%, the midterms 20% each and the final will be worth 40% of the final grade.

## 3 References

There are several good books for quantum mechanics and our library has most of them. For some reason, presently unclear to me, people still want to write books on quantum mechanics. In any case here is a partial list of the few good ones.

- A. Messiah, *Quantum Mechanics I & II*, John Wiley 1958.
- J. J. Sakurai, *Modern Quantum Mechanics*, The Benjamin/Cummings, 1985. (Low price Indian edition is available.)

- ❑ C. Cohen-Tannoudji, B. Diu, F. Laloë, *Quantum Mechanics I & II*, John Wiley (originally published by Hermann, Paris), 2005. (**The various “complements” in this book beautifully illustrate the applications of quantum mechanics**).
- ❑ *Feynman Lectures in Physics vol III*, Addison-Wesley, 1966. (**A must read despite what people might have to say about the “Feynmanisms” in the book**).
- ❑ L. Pauling, E. B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, 1935.
- ❑ L. D. Landau, E. M. Lifshitz, *Quantum Mechanics*, Course of theoretical physics vol. 3, Butterworth-Heinemann, 1958. (**The first 24 pages of this classic are worth reading; read on if you like challenges**).
- ❑ D. A. McQuarrie, J. D. Simon, *Physical Chemistry - A Molecular Approach*, University Science, Chapters 1 - 8 (available as Viva low-priced edition, 1999).

### 3.1 Websites of interest

You might find the following websites useful during the course.

- ① [simons.hec.utah.edu/TheoryPage/](http://simons.hec.utah.edu/TheoryPage/)

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

- ② [ocw.mit.edu/OcwWeb/web/courses/courses/index.htm#Physics](http://ocw.mit.edu/OcwWeb/web/courses/courses/index.htm#Physics)

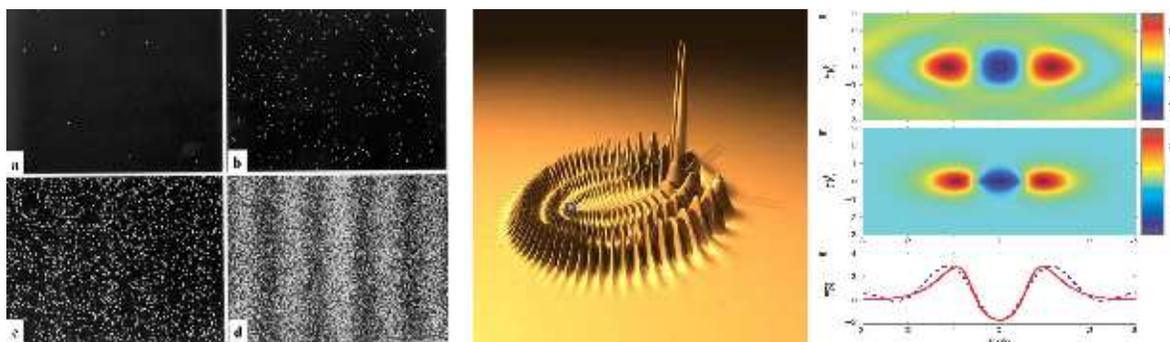
This is the MIT open courseware site and you can find several quantum mechanics courses with readings, lecture notes etc.

- ③ [www.aip.org/history/heisenberg/](http://www.aip.org/history/heisenberg/)

Look into this site for a very nice historical note on aspects of quantum mechanics.

## 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!

