SYLLABUS, Graduate Quantum Chemistry, CHM 767

Semester 2, 2017-2018

Instructor:	W.T. Tysoe, Room 245, Phone (414) 229-5222, E-mail wtt@uwm.edu
Course:	CHM 767, Basic Quantum Chemistry
Venue:	Monday and Wednesday, 3:30-4:45 p.m., Room 195
Prerequisites:	Graduate status and a grade of C or better in Chemistry 562, 564 and Mathematics 234
Assignments:	Problem sets will be given weekly on Monday and collected on the following Monday. Example solutions of these problems will be given. These problems sets are not assigned a grade although comments will be put on the papers. These are for your own benefit and as a help in practicing problems.
Grading:	The course will be graded on the examinations (one final examination). A score will be assigned on the basis of the results in this examination and the final grade will be made on this basis. The class is *not* graded on a curve.
Department Polices:	Information will be posted on bulletin boards which are (a) across from Room 195 of (b) adjacent to Room 164
Textbook:	None: a list of reference texts will be given in the course
Course Outline:	The course will examine the fundamental ideas behind the application of quantum mechanics to chemical systems. Rather than follow an historical approach as is generally done in undergraduate courses, it will treat the ideas of quantum mechanics as a series of postulates that successfully predict experimental results.

1. Introduction to quantum mechanics. Mathematical background, series solutions to differential equations.

2. Description of the postulates of quantum mechanics.

3. "Exact", i.e. analytical solutions to the Schrödinger equation for:
    - Particle in a box
    - Potential step
    - Simple harmonic oscillator
    - Spherically symmetric solutions

4. Use of approximate methods in the solution of the Schrödinger equation using:
    - Time-independent perturbation theory
    - The variation principle
    - WKB theory (a semi-classical theory which is useful for scattering problems. This will be applied to analyzing radioactive decay.)

5. Analysis of angular momentum in quantum mechanics.
    - Commutation and raising and lowering operators
    - Spin angular momentum
    - The addition of angular momentum and the calculation of the resultant eigenfunctions (resulting in the definition of Clebsch-Gordon or Wigner coefficients)

6. Treatment of atoms using quantum mechanics.
    - Indistinguishable particles and the Pauli principle
    - Energies of the helium atom treated using:
        - The variational principle
        - Perturbation theory
        - Self-consistent field methods
    - Correlation energy
    - Exchange energy
    - Hartree-Fock self-consistent field calculations
    - The measurement of the ionization energy from total energy calculations - Koopman's theorem

7. Relativistic effects in quantum calculations of atoms and molecules

8. The Aufbau Principle - putting electrons into multi-electron atoms

9. Quantum mechanics of molecules and bonding:
    - The Born-Oppenheimer approximation
    - Molecular orbital theory applied to H_2^+
    - The generalized Linear Combinations of Atomic Orbitals (LCAO)) Method
    - Mulliken populations
    - The non-crossing rule
    - More accurate calculations - configuration interaction.
    - Less accurate calculations - Hückel theory

10. Elements of density functional theory calculations

11. Application of symmetry in quantum calculations - Group Theory