Syllabus: Mater Structure.

UNIVERSITY OF PUERTO RICO
RÍO PIEDRAS CAMPUS
COLLEGE OF NATURAL SCIENCES
DEPARTMENT OF PHYSICS

Title: Mater Structure
Code: FISI 8105
Number of Credits: 3
Prerequisites: Permission of the Graduate Committee
August 2016

Description

Mater Structure. Development of the basic formalism including the various representations and 'pictures'. Basis of Mater Structure. Basis approaches developed in Mater Structure. Application of tools and methods to analyze structure of simple and complex atomic and molecular systems, and dynamics and structure of biophysical/chemical processes.

Objectives

Through this course, the students will:

- Acquire a basic understanding of the laws of Mater Structure.
- Become proficient with the mathematical formalism of Mater Structure analysis.
- Develop problem-solving skills and strategies in basic Mater Structure in Physics, Chemistry and Biology.
- Communicate effectively a topic pertinent to basic Mater Structure Statements in Physics, Chemistry and Biology

Course Contents and Time Distribution

I. Introduction, Quantum Mechanics Basis (2 wks)
   a) Schrodinger equation;
   b) The particle in the box;.
   c) Stationary and not stationary states;
   d) The perturbation stationary and not stationary theory;
   e) The variation method;
   f) Spin;
   g) The Pauli principle;
   h) Symmetry point groups;

II. Electronic Structure and Spectroscopy of Atoms (3 wks)
   a) Hydrogen atom as model system in atomic spectroscopy.
   c) Multyelectronic atoms;
   d) Single electronic approximation;
   e) Atomic terms. Rassel-Saunders and *j-j* angular momenta coupling schemes;
   f) Fine and hyperfine state structures;

g) Stark effect in atomic states;
h) Zeeman effect in atomic states..

III. Diatomic molecules (2 wks)
a) Systematics of the diatomic molecules terms. .
b) Correlation between atomic terms of the separated atoms with diatomic molecule terms;
c) Borhn-Oppenhimer approximation;
d) Hitler-London method: method of valence scheme (VS);
e) Selection rules for dipole approximation;
f) Molecular Orbital method (MO);
g) H_2^+ ion state structure;
h) Chemical bond. Komton's and exchange integrals;
i) Different bond nature: σ- and π-bonds;
j) Comparison of VS and MO methods.

IV. Electronic Structure and Electronic Spectra of Polyatomic Systems (2 wks)
a) Group Theory;
i) MO method. Hartry-Fock approximation;
j) MO of π-bond systems;
k) MO Huckel method (MOH);
l) MOH for systems with heterogeneous atom;
m) Charge distribution in π-bond systems;
n) Spin density distribution in π-bond systems.

V. Reaction Activity of Molecular systems (1 wks)
a) Perturbation method application to MO;
b) Reactions betweenπ-radicals;
c) Woodward-Hoffman rule. Conservation of orbital symmetry;

VI. Electronic structure and Spectroscopy of Coordinative Inorganic Systems (1 wk)
a) Crystal field theory;
b) MO theory application to coordinative inorganic systems;
c) State structure of coordinative inorganic systems;
d) Spectroscopy of coordinative inorganic systems.

VI. Application of other spectroscopic methods to study of mater structure (4 wks)
a) State structure in low energy region;
b) Radiofrequency and Microwave spectroscopy;
c) State structure in intermediate energy region ($k_BT < E < 1\ eV$);
d) Vibration spectroscopy.

Instructional Strategies
Lectures, problem sets, group discussions, and oral presentations by the students.

Minimum Required Facilities
Traditional lecture room

Student Evaluation
Two partial exams, 3 homework assignments, and oral presentation

Grading System
Standard A to F grading system:
100-90% = A, 89-80% = B, 79-70% = C, 69-60% = D, 59-0% = F.

Bibliography

1. J.N. Murrell, S.F.A. Kittle, J.M. Tedder, Valence Theory, John Wiley and Sons PLD, London – New York - Sydney – Toronto, 1969.
2. L. D. Landau and E. M. Lifshitz, Quantum Mechanics, Fizmatgis, Moscow (1963).
2. William A. Guillory, Introduction to Molecular Structure and Spectroscopy., **Allyn and Bacon; 1st edition (1977)**

Online Resources:

- https://www.unf.edu/~michael.lufaso/chem4627/ch1_solid_state.pdf
- http://scuseria.rice.edu/gau/PBC-Guide.pdf
- https://kar.kent.ac.uk/2546/1/Host-guest.pdf

Rights of Students with Disabilities
UPR complies with all federal and state laws and regulations regarding discrimination, including the Americans with Disabilities Act 1990 (ADA) and the Commonwealth of Puerto Rico Law 51. Students receiving services through Rehabilitación Vocational must contact the professor at the beginning of the semester in order to plan for a reasonable accommodation and any required support equipment according to the recommendations given by the Oficina de Asuntos para las Personas con Impedimentos (OAPI) of the Dean of Students. Likewise, students with special needs that require some type of accommodation must contact the professor.