**Name of the module: Bonding and structure in molecules and solids**

**Number of module: 365-2-9608**

BGU Credits: 3

ECTS credits: 4

Academic year: 2012-2013

Semester: Fall semester

Hours of instruction: 3 hours per week

Location of instruction: will be defined

Language of instruction: Hebrew

Cycle: Second cycle

Position: an advanced course for graduate students of Materials Engineering Department

Field of Education: Materials Engineering

Responsible department: Materials Engineering

General prerequisites: none

Grading scale: the grading scale would be determined on a scale of 0 – 100 (0 would indicate failure and 100 complete success 0 to 100), passing grade is 75.

Lecturer: Prof. Guy Makov

Contact details: room 114, building 59

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Office hours:

TBD

Module evaluation: at the end of the semester the students will evaluate the module, in order to draw conclusions, and for the university's internal needs.

Course Description:

The course will introduce the Schrodinger wave equation and its applications in elementary quantum mechanics. These tools and concepts will be applied to study bonding between atoms and its relation to structure of molecules and solids.

Aims of the module:

Students will be introduced to the elements of quantum mechanics and their application to problems of bonding and structure in materials.

Objectives of the module:

To familiarize students with the Schrodinger wave equation, the nature of its solutions and their physical interpretation. To apply these tools to problems of bonding and structure in materials.

Learning outcomes of the module:

On successful completion of the course the students should be able to:

1. Recognise and identify the elements of Schrodinger wave mechanics.
2. Calculate the expected values of physical quantities.
3. Relate the atomic structure and the periodic table.
4. Relate the bonding characteristics of atoms to the atomic structure.
5. Relate the band structure of solids to the atomic structure.

Attendance regulation: Attendance and submission of assignments is mandatory.

Confirmation: the syllabus was confirmed by the faculty academic advisory committee to be valid on 2012-2013.

Last update: 02.08.2012

Teaching arrangement and method of instruction: lectures, which include examples.

Assessment:

TBD

Work and assignments: will be defined

Time required for individual work: in addition to attendance in class, the students are expected to do their assignment and individual work: at least 2hours per week.

Module Content\ schedule and outlines:

Introduction and motivation of the course, and introduction to wave mechanics, particle in a box (3h)

Formalism of quantum mechanics and harmonic oscillator(3h)

Particle in a 3D box, degeneracy and spherical coordinates (3h)

Hydrogen atom (3h)

The variation method (3h)

Perturbation method (3h)

Spin, many electron atom and the periodic table (3h)

Bonding in diatomics (3h)

Bonding and structure in molecules (3h)

Infinite systems and periodic boundary conditions (3h)

Electronic structure of solids in 3D and band gaps (3h)

Sp bonding in solids (3h)

Free electron theory of metals (3h)

Required reading:

Physical Chemistry, P.W. Atkins and J. de Paula, Oxford University Press, 2010, 9th ed..

Electronic structure of Materials, A. P. Sutton, Oxford University Press (1994).