

302001 – ELECTRONIC STRUCTURE AND PROPERTIES FROM SOLIDS AND INTERFACES

CREDITS: 04 (four) – 60 hours/class

CONTENT:

Approach of solids and crystalline networks through the reciprocal space formalism, Bloch's theorem and band structure. It will be studied the application of formalism using Density Functional Theory and electronic structure calculations with periodic boundary conditions for electronic structure calculations and total energy of extended states in solids; electronic structure and total surface energy; vibrational ways of the crystal lattice. Finally, it will be approached the electronic structure of states located in solids.

SYLLABUS:

1. Solids and crystalline networks:
 - Periodic boundary conditions;
 - Bravais network and network vectors and crystal lattice.
2. Reciprocal space, Bloch theorem and band structure:
 - Reciprocal space vectors;
 - Brillouin area;
 - Bloch's Theorem and its consequences;
 - Extended electronic states and band structure.
3. Density Functional Theory and electronic structure calculations with periodic boundary conditions:
 - Presentation of the Density Functional Theory;
 - Exchange and correlation potentials;
 - Flat and pseudopotential waves.
4. Electronic structure and total energy of extended states in solids:
 - Relations between total energy, geometry and network parameters;
 - Obtaining and analysis of band structure.
5. Electronic structure and total surface energy:
 - Vacuum layer and layer of atoms;
 - Surface energy.
6. Vibrational ways of the crystal lattice:
 - Concept of phonon;
 - Calculation of the phonons structure in simple solid.
7. Electronic structure of states located in solids:
 - Defects and doping;
 - Madelung potential;
 - Models of embedded agglomerates.

BIBLIOGRAPHY:

1. LEVINE, I.N. Quantum Chemistry. Prentice-Hall, 1991.
2. VIANNA, J.D.M.; CANUTO, S.; FAZZIO, A. Teoria Quântica de Moléculas e Sólidos. Livraria da Física, São Paulo, 2004.
3. LESTER, J.N.; BIRKETT, J.W. Microbiology and Chemistry for Environmental Scientists and Engineers. 2.ed. E & FN SPON, 1999.
4. MANAHAN, Stanley E. Environmental Chemistry. 8.ed. CRC Press, 2005.