

**Instructor: Prof. T. Egami** (208 South College, JINS B101 ORNL, egami@utk.edu)

This course is designed for graduate students in materials science, condensed matter physics, chemistry and chemical engineering who are interested in learning physics of real materials. As the advanced materials used or researched today become more complex, simple concepts taught in introductory condensed matter physics courses are no longer sufficient in explaining their functionality. This course starts with the description of the electronic states, bonds and excitations in regular crystals, and extends it to more complex structures including surfaces, interfaces, defects, amorphous and liquid state. It then proceeds to the description of strongly correlated electron systems including magnetism. Advanced experimental methods to study the electronic states and atomic structure are discussed. Students will go through several extended exercises designed to understand the course materials in depth. Basic knowledge of quantum-mechanics and materials physics or condensed matter physics is required.

**Textbook:** *Atomic and Electronic Structure of Solids*, E. Kaxiras (Cambridge University Press, Cambridge, 2003)

**Time and Location:** Wednesday 2:15 – 4:55 pm, Ferris 511.

**Outline:**

1. Electronic states in solids
  - 1-1. Free electron model
  - 1-2. Scattering by a potential
  - 1-3. The concept of pseudo-potential
  - 1-4. Diffraction and band structure
  - 1-5. Density functional theory
  - 1-6. Angle-resolved photoemission spectroscopy (ARPES)
2. Chemical bonds
  - 2-1. Covalent bond and band structure
  - 2-2.  $sp^3$  bonds in Si and Ge
  - 2-3. p-d hybridization in transition metal oxides
  - 2-4. Electron density map determined by x-ray diffraction
3. Electronic excitations
  - 3-1. Optical gap in semiconductor and insulator
  - 3-2. Plasma oscillation and optical response of a metal
  - 3-3. Response function of a metal and Fermi surface nesting
  - 3-4. Friedel oscillation and interatomic potential
  - 3-5. Inelastic x-ray scattering
4. Electron-lattice interaction
  - 4-1. Phonons, second quantization
  - 4-2. Frölich Hamiltonian
  - 4-2. Kohn anomaly

- 4-3. Superconductivity, BCS theory
- 5. Defects and local electronic states
  - 5-1. Impurity states in semiconductors
  - 5-2. Surfaces and interfaces
  - 5-3. Resistivity and impurity scattering
  - 5-4. Electronic structure in matters with nano-scale
  - 5-5. Metal-insulator-transition
- 6. Electronic states in strongly disordered matter
  - 6-1. Concept of percolation
  - 6-2. Disorder and localized states
  - 6-3. Mobility edge
  - 6-4. Electronic states in alloys; split bands
  - 6-5. Coherent potential approximation
  - 6-6. Electronic states in liquids and glasses: Recursion method
- 7. Electron correlation and magnetism
  - 7-1. Exchange interaction
  - 7-2. Stoner magnet, Stoner excitation
  - 7-3. Strong and weak magnetism, half-metallic state
  - 7-4. Magnetism of transition metals and Friedel model
  - 7-5. Hubbard model
  - 7-6. Magnetic impurity and Kondo-resonance
  - 7-7. Friedel sum-rule
  - 7-8. Magnetism of rare earths, indirect exchange
  - 7-9. Heavy Fermion systems
  - 7-10. Fe pnictides superconductors
  - 7-11. Cuprate high-temperature superconductors
- 8. Electrons in biological systems
  - 8-1. Electron diffusion in cells
  - 8-2. Nerve systems

Grading will be based on homeworks, class discussion and two papers. The subject of the papers will be determined by proposal and discussion with the instructor.

Projects:

- 1. Pseudo-potential
- 2. Band structure calculation
- 3. Diagonalization of the electron-phonon Hamiltonian
- 4. Recursion technique for random systems

