GUIDELINES FOR PROJECT PREPARATION

- Select **one project** among those proposed;
- Prepare a **report** that must be sent via mail at least one week before scheduled examination;
- In the report, please **discuss all points** and **clarify all passages**;
- References in brackets can be used as **guideline** for discussion;
- Apart from textbooks, the **scientific papers** are provided in the homepage by using the same label as the project description;
- Apart from problems, any other textbooks or papers selected by student (that can help/complete/improve the discussion) are more than appreciated. A **personal research in scientific literature** is strongly encouraged;
- Feel free to use any **computing systems** (Mathematica, MATLAB or similar) for calculations and graphs preparation. In this case, the **code** must be included in the report.

PROJECT N°1 – VAN HOVE SINGULARITIES

a. Demonstrate the van Hove singularities in density of levels (*Ashcroft-Merlin, Chapter 8, page 143*).
b. Calculate Density of Levels for a Two-Band Model (*Ashcroft-Merlin, Chapter 9, problem 2*).
c. Demonstrate the occurrence of singularities in the Elastic Frequency Distribution of a Crystal (*paper_1*).

PROJECT N°2 – TIGHT BINDING MODEL FOR s- AND p-BANDS

a. Apply the tight-binding model to an s-band arising from a single atomic s-level (*Ashcroft-Merlin, Chapter 10, page 181*).
b. Calculate tight-Binding p-bands in Cubic Crystals (*Ashcroft-Merlin, Chapter 10, problem 2*).

PROJECT N°3 – THE CELLULAR METHOD

a. Discuss the cellular Method for calculating energy bands (*Ashcroft-Merlin, Chapter 11, page 195*)
b. Applicate the Cellular Method to Metallic Sodium as did by Wigner and Seitz (*paper_2*).

PROJECT N°4 – THE KORRINGA-KOHN-ROSTOKER METHOD

a. Discuss Korringa- Kohn-Rostoker method for calculating energy bands in solids (*W. Jones, Theoretical Solid State Physics, page 57)*
b. Discuss the Schrodinger Equation in Periodic Lattices for Metallic Lithium by using KKR Method (*paper_3*).

PROJECT N°5 – BEYOND THE INDEPENDENT ELECTRON APPROXIMATION

a. Describe the Hartree Equation (*Ashcroft-Merlin, Chapter 17, page 330)*
b. Introduce the Hartree approximation *(Ashcroft-Merlin, Chapter 17, page 332)*
c. Derive the Hartree-Fock theory of free electrons *(Ashcroft-Merlin, Chapter 17, page 334).*

PROJECT N°6 – THE EMPIRICAL PSEUDOPOTENTIAL METHOD

a. Describe the Empirical Pseudopotental Method applied to diamond and zinc-blende structures *(M.L. Cohen, Electronic Structure and Optical Properties of Semiconductors, page 20)*
b. Discuss the Self-Consistent and Ab Initio Pseudopotentials *(M.L. Cohen, Electronic Structure and Optical Properties of Semiconductors, page 25)*

PROJECT N°7 – COLLECTIVE EFFECTS IN SOLIDS

a. Determine the classic plasma frequency *(W. Jones, Theoretical Solid State Physics, page 101)*
b. Determine the Static Dielectric Constant *(W. Jones, Theoretical Solid State Physics, page 102)*
c. Determine the Frequency-dependent Dielectric *Constant (W. Jones, Theoretical Solid State Physics, page 105).*

PROJECT N°8 – ELECTROSTATIC SCREENING

a. Discuss the phenomenon of screening as general remarks *(Ashcroft-Merlin, Chapter 17, page 337)*
b. Discuss the Thomas-Fermi Theory of Screening *(Ashcroft-Merlin, Chapter 17, page 340)*
c. Discuss the Lindhard Theory of Screening *(Ashcroft-Merlin, Chapter 17, page 343).*

PROJECT N°9 – SCHRODINGER-POISSON EQUATIONS IN 2D HETEROSTRUCTURES

a. Discuss the Self-Consistent Solution of the Schrodinger and Poisson Equations applied to Quantum Well Heterostructures *(paper_5)*.

PROJECT N°10 – BAND STRUCTURE OF A SINGLE-WALLED CARBON NANOTUBE

a. Starting from the band structure of graphene in tight binding approximation, calculate the electronic band structure of a single-walled carbon nanotube (*paper_4*).

PROJECT N°11 – ELECTRON TRANSPORT IN QUANTUM WIRES

a. Discuss the electron transport properties in quantum wires in the ballistic region and the hot-electron region by solving the Boltzmann equations (*paper_6*).
b. Brief focus on applications: transistors (*paper_6*).

PROJECT N°12 – THEORY OF RANDOM POPULATION FOR QUANTUM DOTS

a. Describe the theory of random population for quantum dots: Carrier capture and recombination. (*paper_5*).

PROJECT N°13 – SILICENE

a. Derive the primitive cell, the Brillouin Zone and the band-structure (Tight-Binding Method) of Silicene, a single atomic layer of silicon, as did in classroom for graphene. (*paper_8*).
