**Course: M.Sc (Physics)**

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| Semester | 4 |
| Paper Number | 20(MPHC4454) |
| Paper Title | Condensed Matter Physics Lab and Computational Condensed Matter Physics |
| No. of Credits | 6 |
| Course description/objective | **Group A:**<br><br>Hands on Experience on the different experimental sets in Condensed Matter Physics (CMP) lab enables the specialization students to understand many of the basic theoretical principles in a better way. They have the unique scope of understanding and developing the sets with the most important component of Error sensing & related analysis.<br><br>**Group B:**<br><br>The objective of this course is to give the students an introduction to the computational techniques used in condensed matter physics. In particular, the package named Quantum Espresso along with the corresponding pseudopotential files are used for this purpose. In the first step, the students will learn the installation procedure. Further they will performcomputation for ‘relax’, ‘vc-relax’ and ‘scf’ calculations. For these, they will know how to write down the input files in which they will link the path to the address where all the pseudopotential files are stored. They are expected to know the meanings of name cards for the pw.exe executable (i.e. ibrav, ntyp, etc.) which are conveniently described in the official page of Quantum Espresso. The main objective of the course is that the students will learn to perform calculations of the bond-length, bond-energy, density of the simple molecules. It is expected that they will be able to visualize the lattice structures after the computations are complete using a suitable software like Xcrysden. Finally, the students should apply the knowledge to calculate the band structure of Silicon. |
| Course Outcome | **Group A**<br><br>CO1: The experiments are spread over a wide spectrum in CMP involving electrical &<br>electronic, optical and mechanical properties of condensed matter.<br>CO2: Some of the experiments are open ended and the students can suggest on procedural, developmental and innovational sides related.<br>CO3: The students are helped with the skill development and thus, they are better trained in seeking fellowship & jobs in future.<br><br>**Group B**<br><br>CO1: Installation of a general software package (like Quantum Espresso/ XCrysden) in Linux/Windows distributions.<br>CO2: Basic idea of ssh client login to remote computing server.<br>CO3: Being able to run a simple code to perform computation in solid-state physics, or similar subjects where many-body interactions are used. |

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| Syllabus | **<u>Group A:</u>**<br>**Condensed Matter Physics Lab [36 Lectures]**<br><br>**List of Experiments:**<br>1. Determination of band gap of a semiconductor sample using UV-VIS spectroscopy.<br>2. Determination of magnetoresistance of a given semiconductor for different magnetic fields.<br>3. Determination of precise lattice parameter and grain size of crystalline materials by X-Ray powder diffractometer.<br>4. To study the temperature dependence of the Hall coefficient for metal/semiconductor.<br>5. Preparation of nanocrystalline powder specimen by chemical route & its size analysis.<br>6. Determination of Band gap of a given semiconductor material by four probe technique.<br>7. Measurement of variation of microhardness of selected specimens.<br>8. Study of colour centers and thermoluminescence of alkali halides.<br>9. Variation of grain size and porosity of sintered/thin film specimens sintered at different temperatures by optical microscope.<br>10. Dispersion relation in a periodic electrical circuit: an analog of monatomic and diatomic lattice vibration.<br>● Hands on experience: Visit to facilities in and around Kolkata and outside Kolkata (subject to availability of accommodation).<br><br>**<u>Group B:</u>**<br>**Computational Condensed Matter Physics [36 Lectures]**<br>Quantum mechanical modeling of materials: Hartree-Fock and Density Functional Theory. Kohn-Sham equation, Exchange-Correlation energy functionals. Hellmann-Feynman theorem. Atomic Pseudopotentials, Basis Sets: Plane Waves and Augmented Basis sets. Plane Wave based DFT calculations. Simplified Approaches to the electronic problem: Tight binding Methods; Slater-Koster approach. Atomistic modeling of materials: Interatomic Potential semi-empirical to many-body system, Classical force fields. Monte Carlo and Molecular dynamics simulations; Hybrid Quantum Mechanics - Molecular Mechanics (QM-MM) method. Ehrenfest, Born-Oppenheimer & Car-Parrinello molecular dynamics. |
| References | **<u>Group A:</u>**<br><br>1. Manuals of the respective experimental set ups<br>2. Introduction to Applied Solid state physics: Richard Dalven, Springer 2012<br>3. Experiments in Condensed Matter Physics: Patel & Sharma, Campus Books International, 2010<br>4. Materials Science: V. Rajendran, Mcgraw Hill 2017 |

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| | **Group B:**<br><br>1. https://www.quantum-espresso.org/<br><br>2. https://github.com/pranabdas/espresso.git<br><br>3. https://github.com/quantumNerd/Quantum-Espresso-Tutorial-2019-Slides.git<br><br>4. https://youtu.be/K2eAHGxCsEg |
| Evaluation | Total: 100<br>**Group A:**<br>CIA: 30 marks (10 (LNB) + 20 (Lab performance))<br>End Semester Examination: 20<br>**Group B:**<br>CIA: 30 marks (10 (LNB) + 20 (CIA Exam))<br>End Semester Examination: 20 |