2/33

# 1605E601

Candidate's Seat No.

**M.Phil. Science Examination**

**Paper-III : Physics EA**

**Time : 3 Hours]** **May-2017** **[Max. Marks : 70**

| | | |
|---|---|---|
| Q.1(A) | Explain in detail, Formation of electronic energy bands in solids. How solids are classified on the basis of these bands? | [07] |
| | OR | |
| | Explain Harrison's construction of Fermi surface in two dimensions. | [07] |
| Q.1(B) | Write short note on a computational tool "Quantum Espresso" | [07] |
| | OR | |
| | Write short note on a computational tool "Gaussian" | [07] |
| Q.2(A) | Discuss three fundamental approximation required for the calculation of band structure. | [07] |
| | OR | |
| | Write schrodinger equation for the conduction electron. Construct orthogonal plane wave, OPWk $=(1-\hat{p})\|k\rangle$. Taking linear combination of OPW, construct wave function of conduction electron Ψk, using such Ψk, show that schrodinger equation reduces to pseudopotential equation with pseudo wave function $\phi k = \sum_q a_q(k)\|k+q\rangle$ and pseudopotential W. [(T+W)ϕk = Ekϕk] | [07] |
| Q.2(B) | Write time dependent schrodinger equation. If $\|k\rangle$ is the state at time t=0 and $\|k+q\rangle$ is state at time t=t, then show that probability of transition from states $\|k\rangle$ to $\|k+q\rangle$ is given by $P_{k,k+q} = (\frac{2\pi}{\hbar})\|\langle k+q\|W\|k\rangle\|^2 n(E)$. Where n(E) is number of states per unit energy range, and $\langle k+q\|W\|k\rangle$ is matrix element of pseudopotential between two states $\|k+q\rangle$ and $\|k\rangle$. | [07] |
| | OR | |
| | Apply perturbation method to obtain solution of time independent schrodinger equation using method of series solution. Write solution for ϕ and W in terms of series. Derive set of equations for different orders of the perturbation. Solving set of equation, calculate total energy E)k). | [07] |
| Q.3(A) | Explain hardness measurement in the annealing treatment in detail. Also show how hardness varies with load respect to as cleaves sample. State your comment. | [07] |
| | OR | |
| | What is hardness? Classify the hardness in terms of load. State different method of hardness measurements and explain Knoop microhardness in detail. | [07] |
| Q.3(B) | Discuss mechanism of creep in detail. | [07] |
| | OR | |
| | State the phase rule and explain binary phase rule. | [07] |

| | | |
|---|---|---|
| Q.4(A) | Describe solid-state reaction technique to synthesize oxides. What is limitation of this route? | [07] |
| | OR | |
| | Describe chemical co-precipitation method of synthesis. Write limitations of present method. | [07] |
| Q.4(B) | Discuss principle and working function of FTIR. List two applications of FTIR. | [07] |
| | OR | |
| | What is use of TGA? Discuss principle and working function of TGA. | [07] |
| Q.5 | Write short Answers: | [14] |
| 1 | Define Fermi energy. | |
| 2 | What is mean by an empty lattice? | |
| 3 | What is LMTO? | |
| 4 | Does 'Wien 2K' is window based or LINUX based? | |
| 5 | What do you mean by optimized Pseudopotential? | |
| 6 | Why one can use perturbation theory in case of Pseudopotential? | |
| 7 | In OPWk method, projection operator in defined for which states? | |
| 8 | What is the disadvantage of plane wave method? | |
| 9 | State the equation of Vickers microhardness. | |
| 10 | What do you mean by cold-worked treatment? | |
| 11 | What is the relation of Brinell Hardness? | |
| 12 | What is difference between endothermic and exothermic reaction. | |
| 13 | List two advantages of Sol-Gel method.[01] | |
| 14 | List two applications of DSC | |

++++++++++++++++++++++++++++BEST OF LUCK++++++++++++++++++++++++++++