Serial No.	Student's Name	Title
P01	Abhinav Kumar	What Drives Charge Ordering in $K_{0.25}CrO_2$, a Microscopic Model
P02	Ashis Kumar Nandy	A magnetic phase diagram for double perovskite oxides
P03	Bipul Rakshit	Stability and the band gap transition study of the layered ZnO
P04	C. Kamal	Ab initio Studies On Properties Of Graphene-like Honeycomb Structures
P05	Dasari Nagamalleswararao	Weak ferromagnetism and magnetization reversal in $YFe_{(1-x)}Cr_xO_3$
P06	Himadri R. Soni	Electronic and Vibrational Properties of Twisted Bilayer Graphene
P07	Hirak Kumar Chandra	What happens to ferroelectricity when you dope carriers?
P08	Jayashree Pan	Half-metallicity and Spin Density Wave State in $BaFeO_3$: A First-principles Study
P09	Jayita Chakraborty	Electronic and magnetic properties of $Ba_3Cu_3Sc_4O_{12}$
P10	Kapil Gupta	Ultra thinfilms: A new route to ferroelectricity
P11	Kaustuv Manna	Experimental Evidences for the Spin-glass ground state in $La_{0.85}Sr_{0.15}CoO_3$ single crystals
P12	M. K. Gupta	Phonons and their Relation with Negative Thermal Expansion in Ag_2O and Cu_2O and Superionic Phase Transition in Li_2O
P13	Narayan Mohanta	Influence of hydrogen impurity in the correlated system GdI_2Hx ($0<x<1$)
P14	Nirmal Ganguli	Predicting the structure and magnetic ground states of the $3d^1$ perovskite oxides $SrVO_3$, $CaVO_3$, $LaTiO_3$, and $YTiO_3$ from ab initio calculations
P15	P K Verma	Density Functional Theory Studies of electrons and phonons in pyrochlores

P16	Prashant Singh	The Harbola-Sahni Potential: A Hybrid Approach towards Band Gap Problem
P17	Rajarshi Tiwari	Incommensurate Magnetic Order and Mott Transitions in Hubbard Model on Anisotropic
P18	Rajiv Kumar Chouhan	Thermal Conductivity and diffusion-mediated localization in $Fe_{1-x}Cr_x$ alloys from first principles
P19	Ravindra Pankaj	A study of cooperative breathing-mode in molecular chains
P20	Santu Baidya	Electronic Structure and Phonons in La_2CoMnO_6: A Ferromagnetic Insulator Driven by Coulomb-assisted Spin-Orbit Coupling
P21	Soumyajit Sarkar	Orbital ordering in FeV_2O_4: Spinel with two orbitally active sites
P22	Sowmya Sathyanarayana Murthy	DFT and beyond-DFT derived tight-binding parameters for $RMnO_3$ using the VASP2WANNIER90 interface
P23	Sudipta Kanungo	Pressure-driven changes in electronic structure of $BiCoO_3$
P24	Swarnakamal Mukherjee	First principles electronic structure study of $CaCu_3M4O_{12}$ (M=Co,Rh,Ir)
P25	S. K. Panda	The Puzzle of NiS