SUMMARIZED PROJECT REPORT

Title of the Project	Period	Funding Agency	Amount (in lakhs of Rs.)	Investigators (PI/Co-PI)	Status	Publications	Manpower trained
Electronic, optical and magneto-optical properties of rare earth compounds	2013-2016	CGCOST, Raipur	5 Lakhs	PI (Dr. S. M. Saini)	Completed	07	01

Achievements:

- Our theoretical investigation for electronic structure of RF_3 (R= Gd and Dy) shows the shifting of the *f* states away from the E_F on inclusion of on-site coulomb interaction i.e. with LSDA+U. It reflects the correct insulating nature of RF_3 in agreement with the experimental data. In Optical properties calculations the low values of reflectivity clearly indicate the transparency of these compounds in the visible and ultra violet region of spectrum in agreement with experimental observations.

- This investigation on RNi_4Si (R = La and Gd) using LSDA+U calculations yield metallic behaviour of both compounds. Analysis of the electronic band structure and density of the states reveals that R-*f* and R-*d* states are present in the conduction bands except spin up Gd-*f* states while Ni-*d* and Si-*s* states are present in the valence bands. Our calculated BS shows that the *f* bands shift towards lower energy as La is replaced by Gd.

- The effect of Si substitution on structural, electronic, optical properties of YNi_4Si- type $RNi_{5-x}Si_x$ (x = 0,1,2) systems suggest that moment at nickel site decreases sharply when nickel is replaced by the silicon. This replacement of nickel with silicon leads to gradual filling of the 3*d* band, as a result of which $N(E_F)$ increases from the value of 1.65 in $DyNi_5$ to 2.16 (states/Ry/spin/unit cell) in $DyNi_3Si_2$.

Novelty and Scientific Outcome:

- There is no theoretical and experimental investigation yet on the electronic and optical properties on RNi_4Si compounds in YNi_4Si- type structure. We expect our work to stimulate the experimentalists to make measurement on RNi_4Si compounds.

- YNi_4Si- type RNi_4Si materials studied in this work are extremely important due to their interesting magnetic and electrical applications in hydrogen storage technology and as adiabatic nuclear cooling agents.

- Study of optical properties i.e. reflectance, optical conductivity, transmittance, of rare earth compounds would give a stringent test whether these materials could be used in many scientific applications i.e. fibre optics, fluorescent lamps and radiation applications and we found that these rare earth compounds are best suitable.