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My Present Research Interests

I am equally interested in Experimental as well as theoretical (mathematical and computational material modeling) research work. At present following research work is running in my lab :

(i) Experimental Material/NanoMaterial Science

In the continuation of my PhD work, I am still involved in experimental research on Material Preparation and characterization studies and solid-state electrochemical device applications viz. solid state batteries. supercapacitor, light emitting electrochemical cell of ionic composites, nano-composites, ionic polymers and polymer nano-composite electrolyte materials. Three scholars have been completed their work in these materials

Dr. Arti Verma – *Characterization analysis of some nanocomposite electrolytes using digital image processing of SEM/TEM images.* –(Awards in 2014).

Dr. Nirbhay Singh- *Investigation on transport properties and material characterization of some nanomaterials for fabrication of supercapacitors* (Awards in 2015).

Homendra Das Sahu- Transport properties study and device applications of some polymer nanocomposite electrolyte system. (thesis submitted recently).

Some PEO based solid electrolytes and nanocomposites were studied experimentally. For detailed structural analysis, image processing of SEM images were performed using java based ImageJ software. Supercapacitors and solid state batteries fabrications and performance studies are the prime objectives of this research. Using SIMULINK, hybrid electric vehicle (HEV) were modeled as an advanced study.

(ii) Theoretical Material/Nano-material Science

- **Mathematical -Modeling** : Mathematical modeling and evaluation of transport properties of some ionic/superionic solids by using space charge depolarization method. Modeling of electrochemical devices viz. solid state batteries, super capacitors and sensors are also in progress. One of the phd thesis of my lab is based on it. Modeling of Light Emitting Electrochemical Cell is under progress.

Dr. B. Keshav Rao - *Modeling of transport properties of some nanoionic materials.* – (Awarded in 2014). MATLAB is used for the modeling of transport properties of some superionic/ionic solids.

- **First principle studies** : Molecular structural, electronic/electrical, mechanical, optical properties analysis of various crystalline/noncrystalline nano-materials, biomaterials, ionic/super-ionic solids and electronic/ionic conducting polymers in context of solid state battery, super capacitor, organic light emitting diode(OLED), light emitting electrochemical cell (LEEC) applications. In these studies density functional based approach implemented in SIESTA, a quantum chemistry based software package is used. For detailed transport properties study NEGF based utility Transiesta is used in present lab. Following students are involved in this approach :

Rachana Singh- Ab-initio modeling and performance study of light emitting electro chemical cells, registered in 2013.

Upma- Studies on the electronic/ionic property of some polymeric biomaterials for medical applications: a density functional approach, registered in 2013.

Structural, Electronic, optical and transport properties of polymers, polymer composites and biomolecules are analysed using first principles before its use in light emitting electrochemical cells and sensors/molecular switches. Graphene structured 2D materials are used as electrodes.

Apart from the above one interactive youtube channel has been launched to help the beginners to associate in this wonderful world of material modeling based on DFT approach. This channel is accepted worldwide by MSc, MTech and PhD scholars to learn SIESTA. The link of channel is :

<https://www.youtube.com/channel/UCb40lsGtuGzECtrtFhQPlvw>