Website Information

Department of Physics

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Research Area	Diluted Magnetic Semiconductors, Spintronics, Strongly Correlated Electron Systems, 2D Magnetic Materials, Magnonics, Thermoelectric Materials
Publications (Past 5 years)	1. **D. Manikandan**, R. K. Yadav, K. Ramesh, R. Murugan, D. W. Boukhvalov, A. K. Yadav, R. Gupta, Dopant-activated magnetism and local structure properties of cubic shape Co, Mn: In_2O_3, ***Mater. Sci. Semicond. Process*** 2023, **168**, 107818. 2. **D. Manikandan**, K. Ramesh, R. Murugan, D. W. Boukhvalov, M. Senthil Pandian, P. Ramasamy, Morphology controlled synthesis of Fe and Mn co-doped In_2O_3 nanocubes and their dopant-atom effects on electronic structure and magnetic properties, ***J. Magn. Magn. Mater***. 2022, **560**, 169547. 3. **D. Manikandan**, R. Murugan, Genesis and tuning of ferromagnetism in SnO_2 semiconductor nanostructures: comprehensive review on size, morphology, magnetic properties and DFT investigations, ***Prog. Mater. Sci.***, 2022, **130**, 100970. 4. **D. Manikandan**, R. Murugan, D. W. Boukhvalov, K. Ramesh, V. Sivasubramani, M. Senthil Pandian, P. Ramasamy, Effect of vacancy defects on electronic structure and ferromagnetism in pristine In_2O_3 nanostructures: An experimental study and first-principles modeling, ***Mater. Res. Bull***. 2022, **152**, 111853**.** 5. **D. Manikandan**, I. S. Zhidkov, A. I. Kukharenko, S. O. Cholakh, E. Z. Kurmaev, R. Murugan, Investigation on electronic structure and magnetic properties of Co and Mn incorporated nanoscale SnO_2, ***Appl. Phys. A***, 2020, **126**, 545. 6. J. Ho, T. D. Boer, P. M. Braun, B. Leedahl, **D. Manikandan**, R. Murugan, A. Moewes, Origin and control of room temperature ferromagnetism in Co, Zn-doped SnO_2: Oxygen vacancies and their local environment, ***J. Mater. Chem. C***, 2020, **8**, 4902. 7. D. E. J. Ruth, R. A. U. Rahman, **D. Manikandan**, L. Venkidu, B. Sundarakannan, P. Schmid-Beurmannc, P. Zhou, G. Srinivasan, R.

	Murugan, Room temperature magnetoelectric coupling in Fe-doped sodium bismuth titanate ceramics, ***J. Alloy. Compd.,*** 2020, **830**, 154679. 8. **D. Manikandan,** A. K. Yadav, S. N. Jha, D. Bhattacharyya, D. W. Boukhvalov, R. Murugan, XANES, EXAFS, EPR and first-principles modeling on electronic structure and ferromagnetism in Mn-doped SnO_2 quantum dots, ***J. Phys. Chem. C****,* 2019, **123**, 3067. 9. D. W. Boukhvalov, **D. Manikandan**, I. S. Zhidkov, A. I. Kukharenko, S. O. Cholakh, E. Z. Kurmaev, R. Murugan, Effect of doping and annealing on the electronic structure and magnetic properties of nanoscale Co and Zn co-doped SnO_2: an experimental study and first-principles modeling, ***J. Alloy. Compd.****,* 2019, **799**, 433.
Profile Links Scopus and Orcid	**Scopus Author ID**: 56167631400 **Orcid :** https://orcid.org/0000-0001-5434-0631
Research Activities (Write about your best research results max of 2-3 pages including diagrams)	My current research is oriented towards oxide-based diluted magnetic semiconductors, 2D magnetic materials, and strongly correlated electron systems for the spintronics and magneto-electronics device applications. On the other hand, I am further working on the thermoelectric materials. **1. Emerging Nanoscale Diluted Magnetic Semiconductors for Spintronics Devices Applications** (a) SnO_2-based Diluted Magnetic Semiconductor Quantum Dots The ultimate focus of the research work was to elucidate the origin and control of room temperature ferromagnetism in SnO_2-based DMS by using various experimental techniques and first-principles modeling. In this regard, single-phase SnO_2 and Mn doped SnO_2 quantum dots (QDs) were investigated under the influence of dilute Mn concentration. SnO_2 and Mn doped SnO_2 (2%, 4%, 6%, and 10%) quantum dots (QDs) synthesized by high-pressure microwave synthesis technique were investigated. Single-phase with tetragonal rutile structure of synthesized QDs were substantiated from the powder X-ray diffraction (PXRD), Raman, and selected area electron diffraction (SAED) analysis. The formation of spherical shape and uniform size of the synthesized quantum dots was visualized using high-resolution transmission electron microscope (HRTEM) micrographs. The estimated particle size of the synthesized QDs was in the range of 2.7-2.4 nm. Results of X-ray photoelectron spectroscopy (XPS) and electron energy loss spectroscopy (EELS) revealed that at lower doping concentrations (2% Mn) the oxidation state of Mn mostly as +2 and higher doping concentration (10% Mn) leads to multiple configurations of Mn (Mn^{2+} and Mn^{3+}). Field-dependent magnetic properties of synthesized QDs indicated the room temperature ferromagnetism (RTFM) (Figure 1). Results of X-ray absorption near edge structure (XANES) (Figure 1) showed that the predominance of Mn^{3+} at lower concentrations and higher Mn dopant concentration leads to the predominance of Mn^{3+} along with Mn^{2+}. Extended X-ray absorption

fine structure (EXAFS) indicated that the first Mn-O bond length decreased for the 2, 4, and 6% Mn-doped QDs. Conversely, the bond length of 10% Mn-doped SnO_2 QDs was slightly increased. For a deep understanding of the electronic structure and magnetic properties of synthesized QDs first-principles modeling (Figure 2) were used and the theoretical results were correlated to the experimental findings.

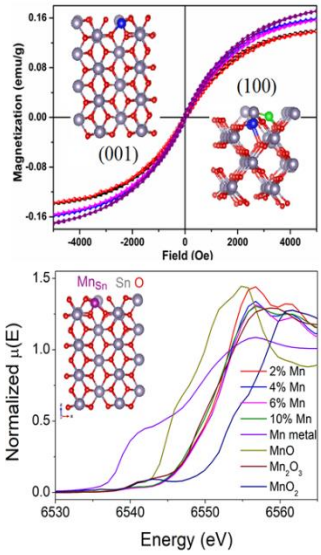

Figure 1

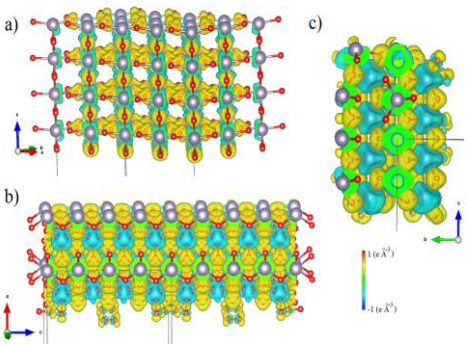

Figure 2

In order to further explore the origin of ferromagnetism and to enhance the magnetic properties of the SnO_2 system, the focus was oriented on double doping which contains both magnetic and nonmagnetic elements.

(b) In_2O_3-based Diluted Magnetic Semiconductors

The origin and control of room temperature ferromagnetism in In_2O_3-based diluted magnetic semiconductors (DMS) were systematically investigated via a combination of experimental techniques and first-principles modeling**.** The influence of annealing and doping effects on the physical properties of In_2O_3 nanostructures was systematically investigated. In this way, single-phase pristine In_2O_2 nanorods and porous nanoparticles were prepared by the hydrothermal-annealing method. Single-phase cubic crystal structure of the prepared samples was established via PXRD, Raman, and SAED analysis. More interestingly, the change in morphology from rectangular nanorod shape to porous nanoparticles (Figure 3) was visualized at higher annealing temperature using a high-resolution transmission electron microscope HRTEM. The formation of the inherent vacancy-like oxygen vacancies and regulation in electronic structure was evidenced via XPS and Raman analysis. Magnetic measurements demonstrated the RTFM in the prepared nanorods and nanoparticles. The combination of experimental and first-principles modeling established the origin of observed RTFM in the prepared nanorods and nanoparticles was associated with the formation of inherent defects. Further, a theoretical model (Figure 4) was proposed to explain the observed RTFM and semiconductive electronic structure.

Additionally, the appropriate magnetic and non-magnetic transition metals were doped to improve the magnetic properties. The prepared sample's local structure properties were studied using the XANES and EXAFS. Single-phase SnO_2 and In_2O_3-based DMS with RTFM were optimized to achieve potential spintronic materials suitable for the next generation of storage and logic devices.

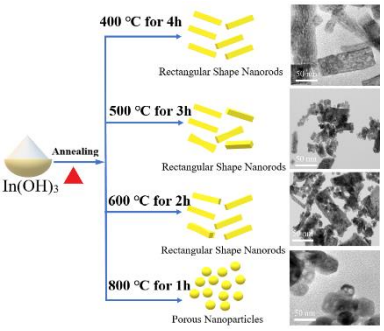

Figure 3

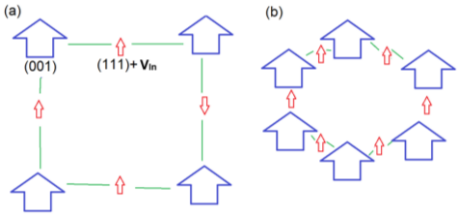

Figure 4

2. Study of Spin and Orbital Magnetism in Frustrated Spinel Vanadates

The strongly correlated electron systems (SCES) have drawn particular interest recently for their challenging fundamental properties and coexisting multiple long-range orders (charge, magnetic, and orbital order). The family of spinel vanadates (AV_2O_4) belongs to SCES systems where strong correlation, geometric frustration, and complex spin texture of the fundamental latticework in tandem. In this way, the structural and magnetic properties of frustrated spinel vanadates like MnV_2O_4 and CoV_2O_4-based systems were explored. The pristine and TM-incorporated MnV_2O_4 samples were prepared using a conventional solid-state synthesis technique. On a wide-ranging vision, the impact of TM incorporation on the structure, electronic structure, and magnetic ground state of the MnV_2O_4 was explored via complementary experimental and theoretical approaches. All the prepared samples revealed the cubic structure with space group $Fd\bar{3}m$. Interestingly, the pristine sample exhibited paramagnetic to ferrimagnetic transition beside cubic to tetragonal structural transition at a low-temperature regime. Furthermore, Single-phase pristine and TM-doped CoV_2O_4 of different doping concentrations were prepared via solids state reaction technique. The monophase samples indicated typical magnetic low-temperature transition and regulation in electronic structure. The electronic band structure and magnetic properties were further simulated for the fundamental understanding of exotic magnetic properties. These investigations were likely to provide a deep understanding of the origin of spin canting and orbital ordering in spinel vanadates.

Collaborations	▪ Prof. Alexander Moewes, Department of Physics and Engineering Physics, University of Saskatchewan, Canada.

	▪ Prof. Ernst Z. Kurmaev, M. N. Mikheev Institute of Metal Physics of Ural Branch of Russian Academy of Sciences, Yekaterinburg, Russia. ▪ Dr. Danil W. Boukhvalov, College of Science, Institute of Materials Physics and Chemistry, Nanjing Forestry University, China. ▪ Prof. Rajeev Gupta, Materials Science Programme, Indian Institute of Technology, Kanpur, India. ▪ Dr. K. Ramesh, Department of Physics, Indian Institute of Science, Bengaluru, Karnataka, India.
Awards and Recognition	o Institute Postdoctoral Fellowship, Materials Science Programme, Indian Institute of Technology Kanpur, India (from June 2022-June 2024). o Basic Science Research-Junior/Senior Research Fellowship (2015-2019), University Grants Commission, India. o Summer Internship Fellowship (2011), Indian Institute of Science, Bengaluru, India.