- Virginia Commonwealth University, Richmond, USA (2001-02)
- University of New South Wales, Sydney, Australia (2016)

Research Areas :

- Materials simulation and design using first-principles Density Functional Theory
- Energy Materials, Hydrogen storage, Photocatalytic materials.
- Graphene and related 2-dimensional nanostructures.
- Spintronics Materials based on Diluted Magnetic Semiconductor (DMS) and Diluted Magnetic Oxide (DMO)
- Topological materials and quantum structures
- *Ab initio* molecular dynamics of metallic and semiconducting clusters
- Phase stability and configurational thermodynamics of binary alloys.
- Cohesive, Electronic and Magnetic properties of ordered and disordered condensed systems
- Electronic properties of epitaxial metal/semiconductor and metal/ceramic interfaces, metallic multilayers and polytypes.
- Electron momentum density distributions in solids (using Compton Scattering and Positron Annihilation).

Awards & Recognitions :

- ACCMS International Award, by the Asian Consortium on Computational Materials Science, in recognition of high level research work on Computer Aided Design of Materials.
- Chair of Psik-2020 Theme Symposium (2020) on "Materials for Energy", Lausanne, Switzerland. (Postponed to 2022 due to Covid19)
- Distinguished Speaker, Wright Patterson Air Force Base, Ohio, USA (2017)
- Guest Editor of J. Phys. : Cond. Matter (JPCM) Special Issue *"Ordering, Segregation and Order-Disorder Transition in Alloys" (2020-21)*
- Chairman, MRSI Subject Group on Computational Materials Science (since 2010)
- President, Indian Association for the Physics Teachers (IAPT), RC-15 (since 2016)
- Fellow, West Bengal Academy of Science & Technology (2005)

Guiding Students :

- Ph.D. students (principal supervisor) : 10 (awarded), 1 (currently doing PhD)
- Ph.D. students (co-supervisor) : 3
- Integrated M.Sc students : 1
- M.Tech students : 2
- Post-docs : 3

Publications *[h-index 28, i-index 69, total citation ~3000]* ★ ¶

- 150 (vide complete list of publications), which includes
- 10 Review Articles and Book Chapters
- 20 Papers published in books and conference volumes
- 3 Edited Volumes

Invited talks :

- More than 50 in International Meetings outside India
- More than 100 in National and International Meetings held in India

Lecture Courses Delivered :

- Micro-credit courses on DFT in IIT Kharagpur (2020), IIT Mandi (2019)
- Nanomechanics Course, Centre for Theoretical Studies, IIT Kharagpur (2019)

- Physics of Materials (B.Tech., Final year), IIT Kharagpur (2018)
- Atomistic Modeling of Materials (B.Tech., Final year), IIT Kharagpur (2018)
- Short Course on Computational Materials Science, SRM University (2017)
- Electronic Structure and Properties of Low Dimensional Systems and Quantum Structures, IIT Kharagpur (2016)
- PhD Course Work on Electronic Structure and Properties of Materials, IACS Kolkata (2015)
- Refresher Course on Interdisciplinary research using Nanoscience and Nanotechnology, Jadavpur Univ. (2015)
- Refresher Courses in Calcutta Univ. (2009-14), Pune Univ (2020), IIT Indore (2021)
- Special Elective Course on "Tensor properties of Solids" Science College, Calcutta Univ. (2011)
- UGC Sponsored Network "Electronic Structure of Materials: Density Functional Approach", Institute of Radio Physics & Electronics, Calcutta Univ. (2010)
- Lecture courses on Solid State Physics, Quantum Mechanics, Mathematical Methods and Statistical Analysis, BARC Training School for Post-M.Sc. Physics students (1980 – 1997)

Services in different national and international committees :

- Organized Pan-IIT Webinar series on "Materials Simulation : A Virtual Guided Tour" (May 2020)
- Co-organize the CMS Session (V5H1S5) of VAIBHAV Global Summit organized by Govt of India (Oct '20)
- Organized Theme Session on Computational Materials Science in 2nd Indian Materials Conclave, Kolkata (February, 2020)
- Coordinator of Micro-credit course on "Time-dependent Density Functional Theory & Its Applications", IIT Kharagpur (Jan 2020)
- Acted as a Member of the Review Committee for preparing the 'Road Map' for Srinivasa Ramanujan Institute for Basic Sciences SRIBS, Kottayam (July '18)
- Member, Board of Studies of Physics Department of St. Xavier's College, Barasat Govt. College, (responsible for formulation of academic syllabus of undergraduate & post-graduate courses)
- Member of Academic Advisory Board of Jagadish Bose National Science Talent Search (JBNSTS) 2013.
- Member Steering Committee, Asian Hydrogen Storage Materials (2011)
- Mentor for Innovation of Science Pursuit for Inspired Research (INSPIRE) programme of the DST since 2005
- Chairman, MRSI Subject Group on Computational Materials Science since 2000.
- Founding Member of Asian Consortium for Computational Materials Science (ACCMS) since 2000.
- Member, ICTP-OEA Network on Metals and Alloys (1987-90)

Services in editorial boards of journals :

- Associate Editor, International Journal of Modern Physics B (IJMPB), World Scientific (Since 2010)
- Associate Editor, Modern Physics Letters B (MPLB), World Scientific (Since 2010)
- Member Editorial Board, International Journal of Computational Materials Science & Engineering (IJCMSE), World Scientific, Singapore (Since 2010)
- Guest Editor, Materials Transaction Special Issue on "Clusters & Nanomaterials" (2007)
- Guest Editor, J. Phys. Condensed Matter Special Issue on "Ordering, Segregation and Order-Disorder Transition in Alloys" (2020)
- Reviewer of several International Journals on Physics, Chemistry & Materials Science,
  - Phys. Rev. B, Phys Rev. Lett. ACS Nano, J. Phys. Chem. C, European Phys. J.,
  - Physica E, Phys. Stat. Sol., AIP Advances, Int. J. Hydrogen Storage, etc.

Major projects :

- IACS-BARC Project on Quantum Structures and Phenomena (IBIQuS), (2009 - 2017) from Dept of Atomic Energy, under the 12th Five year plan, This Experiment-cum-Computation project was jointly with Prof. B.N. Dev (IACS)
- VR-SIDA Project on "Hydrogen Storage Materials for Energy Applications", with Uppsala University, Sweden (2008-2012)
- Coordinated Research Project on "Spintronics Materials", Board of Research on Nuclear Sciences (BRNS) (2006-2010)
- DMRL Project on Development of Computational Methodologies for Thermodynamics of Multicomponent Systems using Cluster Variation Method (2004-2006)