Prof. G.P. Das

Prof. G.P. Das is a Condensed Matter Physicist cum Materials Scientist, who is well known for his contributions in the emerging field of materials modeling, simulation and design. He is currently working as a Visiting Professor in the Indian Institute of Technology (IIT) Kharagpur where he is associated with the Dept. of Metallurgical & Materials Engineering jointly with the Dept. of Physics and the School of Nano Science & Technology. Prior to this, he served as a senior professor in the Indian Association for the Cultivation of Science (IACS) Kolkata and as senior scientist in Bhabha Atomic Research Centre (BARC) Mumbai. He has published over 150 original research papers in international journals and book chapters in diverse areas such as alloys, intermetallics, nanostructures, energy materials, semiconductor devices, spintronics materials and various kinds of quantum structures. Apart from this, he has delivered invited talk in more than 100 international conferences all over the world. Prof. Das had served as visiting scientist in Max Planck Institute Stuttgart (Germany), Virginia Commonwealth University, Richmond (USA), Institute of Materials Research, Sendai (Japan), International Centre for Theoretical Physics, Trieste (Italy), and University of New South Wales (Australia). He has successfully steered several research programmes nationally and internationally.

Educational Degree(s) :

- B.Sc. in Physics 1973, St. Xaviers' College, Calcutta University (Ist class).
- M.Sc. in Physics 1975, University College of Science, Calcutta (Ist class).
- PhD in Physics 1986, Bombay University
- Postdoctoral Research 1987-1989 Max Planck Institute for Solid State Research, Stuttgart, Germany

Positions held :

- Visiting Professor, IIT Kharagpur (June 2018 – present)
- Senior Professor, Dept. of Materials Science, IACS, Kolkata, 2006 – 2018
- Professor, Dept of Materials Science, IACS, Kolkata 2004 – 2006
- Adjunct Professor, IIEST Shibpur (2010), Distinguished Visiting Professor of PSG Institute of Advanced Studies, Coimbatore (2014), Adjunct Faculty, MAKAUT, WB (2019),
- Senior Scientist, Bhabha Atomic Research Centre, Mumbai, 1989-2004
- Scientific Officer, Bhabha Atomic Research Centre, Mumbai, 1978-1989

Long- as well as Short- term Visiting Positions abroad :

- Max Planck Institute for Solid State Research, Stuttgart, Germany (1987-89, 1992),
- International Center for Theoretical Physics (ICTP), Trieste, Italy (1988-89)
- University of Groeningen, The Netherlands. (1989)
- Institute of Materials Research, Tohoku University, Sendai, Japan. (2010, plus several short term visits during the past decade)

- 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)