

## CV of Prof. G.P. Das

Department of Metallurgical & Materials Engineering,  
jointly with Department of Physics and School of Nano Science & Technology,  
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Prof. G.P. Das is condensed matter physicist with research interests spanning a wide cross-section in the area of solid state physics and materials science, particularly on first principles investigation of electronic and magnetic properties of alloys, interfaces, clusters, and nanostructured materials (*fields of specialization and expertise appended below*). He is presently working as a visiting professor in the Department of Metallurgical & Materials Engineering, jointly with the Department of Physics and the School of Nano Science & Technology. Earlier he had worked as a senior research scientist in Bhabha Atomic Research Centre Mumbai (till 2004), before joining the Indian Association for the Cultivation of Science (IACS) Kolkata as a senior professor in the Department of Materials Science. He graduated from Calcutta University and after obtaining his Ph.D. in Physics from Bombay University, he did his post-doctoral research in the Max Planck Institute for Solid State Research in Stuttgart. He also served as visiting scientist in several institutes abroad such as Max Planck Institute Stuttgart (Germany), Virginia Commonwealth University, Richmond (USA), Institute of Materials Research, Sendai (Japan), ICTP Trieste (Italy), University of New South Wales (Australia) etc.

Prof. Das has nearly four decades of research cum teaching experience. He has taught in PG as well as UG level, and is also well known for his pedagogic as well as popular level lectures in condensed matter physics, materials science, nano-science and energy science. For several years he has been serving as a mentor in DST's INSPIRE programme, in JBNSTS programme etc. Prof. Das has authored and co-authored more than 150 research papers, including a number of review articles and book chapters. He has guided (and is currently guiding) as principal supervisor 10 PhD students, 4 M.Tech / M.Sc students and 3 post-doctoral fellows. He was also instrumental in co-supervising 3 PhDs. He has delivered more than 70 invited talks in International Conferences and Workshops. He has successfully completed several major projects funded by DRDO, DAE, VR-SIDA and other agencies. These are in the areas of (a) multiscale modeling of alloys (b) simulation and design of spintronics materials and (c) hydrogen storage materials based on complex chemical hydrides and nanostructures. The most recent project (jointly with Prof. B.N. Dev) being the IBIQuS Project on Quantum Structure, funded by the Dept of Atomic Energy under the 12<sup>th</sup> Five-year plan.

Prof. Das is the recipient of the MRSI Silver Jubilee Medal Award in 2014, ACCMS Award in 2013 and he is a Fellow of the West Bengal Academy of Science & Technology. Prof. Das has been selected as an Honorary Adjunct Professor in Bengal Engineering & Science University (BESU) and also as a Distinguished Visiting Professor in the PSG Institute of Advanced Studies. He is currently acting as chairman of the MRSI subject group on Computational Materials Science, serving as a member of DST's Project Management Board on Supercomputing Facility, and is also member of the steering committee of Asian Consortium for Computational Materials Science (ACCMS) and of Asian Hydrogen Storage Materials (ASHM) initiative.

## Curriculum Vita of Prof. G.P. Das

### 1. PERSONAL

- Date of Birth : 31 May, 1954
- Marital Status : Married
- Present Position : Visiting Professor
- Postal Address : Departmental of Metallurgical & Materials Engineering  
Jointly with Department of Physics and School of Nano Science & Tech  
Indian Institute of Technology,  
Kharagpur-721302, India
- E-mail address : [gpdas@metal.iitkgp.ac.in](mailto:gpdas@metal.iitkgp.ac.in); [gourpdas@gmail.com](mailto:gourpdas@gmail.com)
- Phone No. : 03222-281900 (Off); 9433192231 (Cell);
- FAX No. 03222-282280

### 2. ACADEMIC

- B.Sc. in Physics 1973, St. Xaviers' College, Calcutta University (Ist class).
- M.Sc. in Physics 1975, University College of Science, Calcutta (Ist class).
- Ph.D. in Physics 1986, University of Bombay.

### 3. POSITIONS HELD

#### Current Position :

Visiting Professor, Department of Metallurgical and Materials Engineering  
Jointly with Department of Physics and School of Nano Science & Technology

#### Previous Positions :

- Senior Professor, Dept. of Materials Science, IACS, Kolkata, 2006 – 2018
- Professor, Dept of Materials Science, IACS, Kolkata 2004 - 2006
- Visiting Scientist, Virginia Commonwealth University 2001-02 (on deputation leave).
- Post-doctoral Fellow, Max Planck Institute for Solid State Research, Stuttgart, 1987-89
- Scientific Officer, Bhabha Atomic Research Centre, Mumbai, 1978-2004

### 4. TEACHING COURSES & STUDENTS SUPERVISED

#### Lecture Courses Delivered :

1. Physics of Materials (B.Tech., Final year), IIT Kharagpur (2018)
2. Atomistic Modeling of Materials (B.Tech., Final year), IIT Kharagpur (2018)
3. Short Course on Computational Materials Science, SRM University (2017)
4. Electronic Structure and Properties of Low Dimensional Systems and Quantum Structures, IIT Kharagpur (2016)
5. PhD Course Work on Electronic Structure and Properties of Materials, IACS Kolkata (2015)
6. Refresher Course on Interdisciplinary research using Nanoscience and Nanotechnology, Jadavpur Univ. (2015)
7. Refresher Courses Science College, Calcutta Univ. (2014, 2011, 2009)
8. Special Elective Course on “Tensor properties of Solids” Science College, Calcutta Univ. (2011)
9. UGC Sponsored Network “Electronic Structure of Materials: Density Functional Approach”, Institute of Radio Physics & Electronics, Calcutta Univ. (2010)
10. Lecture courses on Solid State Physics, Quantum Mechanics, Mathematical Methods and Statistical Analysis, BARC Training School for Post-M.Sc. Physics students (1980 – 1997)

#### PhD thesis supervised :

Supervised 10 PhD students as main supervisor (7 completed, 3 ongoing), 3 (as co-supervisor) and 4 M.Tech students, plus several short term summer course students for their M.Sc. thesis.

### **PhD Thesis completed (as main supervisor) :**

1. Saurabh Ghosh (2011) "First Principles Investigation of Nanostructured Diluted Magnetic Semiconductors and Oxides"
2. Saswata Bhattacharya (2011) Thesis title : "First-principles design of bulk and nano-materials for hydrogen storage",
3. Amrita Bhattacharya (2013) Thesis title "First principles study of functionalized graphene and its derivatives",
4. Sonali Barman (2014) Thesis title : "Effects of doping and alloying on structural, electronic and magnetic properties of novel clusters: A first-principles study"
5. A.H.M. Abdul Wasey (2016) Thesis title : "Studies of Two-Dimensional Quantum Structures using First Principles Density Functional approach"
6. Soubhik Chakrabarty (2017, to be submitted) Thesis title : "Functionalization of Carbon based Planar Nanostructure: A first-principles study"
7. Paramita Banerjee (2017, to be submitted) Thesis title : "Nanostructured Materials for Storage of Hydrogen and its Utilization in Fuel Cells : A first-principles study"

### **Ph.D. Thesis currently guiding (as main supervisor)**

8. Tisita Das (since 2013) Currently working on "Electronic Structure and Properties of Low Dimensional Carbon Systems"
9. Moumita Mukherjee (since 2014) Currently working on "Study of Graphene – Organic Composite with Optoelectronic Applications".
10. Abhirup Roy Karmakar (since 2018) just started after my joining IIT Kharagpur

### **PhD Thesis co-supervised (while working in BARC)**

11. Dr. Hemant G. Salunke (BARC, Technical Physics Division, 1997) Thesis title : "Electronic Structure and Superconductivity in Zr based Transition Metal Intermetallics"
12. Dr. Ashok Arya (BARC, Materials Science Division, 1998) Thesis title : "First principles studies on phase stability and order-disorder transformation in Al-Li & Ni-Mo"
13. Dr. Nandan Tandon (Pune University, 2009) Thesis title : "Studies of Electronic Structure and Magnetism in Transition Metal Doped GaN and CdTe"

### **Post-doctoral Researchers :**

1. Dr. Satadeep Bhattacharya (2005-06)
2. Dr. Ranjit Thapa (2011-12),
2. Dr. Deepanjan Dutta (2013)

### **M. Tech. / M.Sc. Project Thesis Supervised :**

1. Mr. Kuntal Talit, M.Tech. (2010)
2. Mr. Subir Majumder, M.Tech. (2011)
3. Mr. Sujit Narayanan, M.Sc. (2012)
4. Mr. Aritra Ghosh, M.Sc. (2013)

### **5. AWARDS, HONOURS AND RECOGNITIONS**

- Distinguished Invitee, Air Force Research Laboratory (AFRL), Dayton, USA (2017)
- Associate Editor, Modern Physics Letter B (2016)
- Recipient of Materials Research Society of India (MRSI) Silver Jubilee Medal (2014)
- Recipient of Asian Materials Science Award of the Asian Consortium for Computational Materials Science (ACCMS) in 2013.
- Appointed as External Expert Member for the India-EU collaborative project on Computational Materials Science (2013).

- Recipient of VR-SIDA Swedish Project on Hydrogen Storage Materials for Energy Applications (2012-present).
- Member Steering Committee, Asian Hydrogen Storage Materials (2011)
- Guest Editor, Materials Transaction Special Issue on Clusters & Nanomaterials (2007).
- Member, DST-FIST Program Subject Expert Committee on Chemical Science
- Chair, IUMRS-ICAM-2007 Theme Symposium on Computational Materials Science.
- Member, Editorial Board, International Journal of Computational Materials Science & Engineering (IJCMSE)
- Member of Executive Committee of '*Asian Consortium for Computational Materials Science*'
- Recipient of Materials Research Society of India (MRSI) Medal (2000).
- Member of the International Advisory Committee of Psi<sub>k</sub> ( $\psi_k$ ) European Network Conference Schwaebisch Gemuend (1996 & 2000).
- Chairman, Computational Materials Science Subject Group of MRSI (1999-present)
- Selected as Speaker of Theoretical Physics Seminar Circuit (1993) .
- Awarded Max Planck Fellowship (1987 – 1989) .
- Awarded National Merit Scholarship (1970).

## 6. FIELDS OF SPECIALIZATION AND EXPERTISE

- First principles electronic structure (mainly DFT based) of alloys, interfaces, multilayers, clusters, nanostructures
- Graphene and related 2-dimensional systems, e.g.h-BN sheet, Silicene, TM-dichalcogenides
- Hydrogen storage materials : from Bulk Complex Hydrides to Functionalized Nanostructures
- Spintronics Materials based on Diluted Magnetic Semiconductors and Oxides
- *Ab initio* molecular dynamics of metallic and bimetallic clusters.
- Phase stability and configurational thermodynamics of binary, and ternary metallic alloys.
- Interface indeed properties of epitaxial metal/semiconductor and metal/ceramic interfaces.
- Electron momentum density distributions in solids (Compton Scattering & Positron Annihilation)

## 7. INSTITUTIONS VISITED (LONG- & SHORT-TERM)

- Max Planck Institute for Solid State Research, Stuttgart, Germany (1987-89)
- Virginia Commonwealth University, Richmond, USA (2001-02)
- Institute of Materials Research, Tohoku Univ, Sendai, Japan (2006).
- University of New South Wales, Sydney, Australia (2016)
- University of Groeningen, The Netherlands.
- International Center for Theoretical Physics (ICTP), Trieste, Italy; delivered lecture series on Electronic Structure of Alloys and Intermetallics

## 8. MEMBERSHIPS OF PROFESSIONAL SOCIETIES

- Indian Physics Association (IPA).
- Materials Research Society of India (MRSI)
- Indian Physical Society (IPS).
- Indian Association of Physics Teachers (IAPT)
- American Physical Society (APS)
- Japan Society for Promotion of Science (JSPS)

## 9. PROFESSIONAL SERVICES

- Associate Editor, Modern Physics Letter B (2015 – Present)
- Member, Editorial Board, International Journal of Computational Materials Science & Engineering (2011 – Present)
- Reviewer of several International Journals on Physics, Chemistry and Materials Science, e.g. 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. And I have peer reviewed about 50 papers during the last 10 years.

- Member, Board of Studies (Physics), St. Xavier's College (Deemed University), Barasat Government College,
- Member, Expert Committee for Nanoscience Programme at IGNOU (2009)
- Member, ICTP-OEA Network on Metals and Alloys (1987-90).

#### **10. ADMINISTRATIVE RESPONSIBILITIES**

- Honorary President, IAPT RC15, Indian Association for Physics Teachers (2016 – Present)  
Responsibilities : Organizing Schools and Workshops for Physics Teaching in West Bengal & neighboring areas
- Head, Materials Science Dept., Indian Association for the Cultivation of Science (2014-2016)  
Responsibilities : Administration and Financial Planning of the Departmental Scientific Activities
- Member, DST-FIST Program Subject Expert Committee on Chemical Science (2011 – 2015)  
Responsibilities : Screening and Evaluation of FIST proposals on Chemical sciences
- Member, International Advisory Committee, Asian Consortium for Computational Materials Science – ACCMS (2000 – Present) Responsibilities : Planning ACCMS Meetings in different Asian countries / regions
- Chairman, MRSI Subject Group on Computational Materials Science (1999 – Present);  
Responsibilities : Steering national level activities for promoting CMS

#### **11. OUTREACH ACTIVITIES**

- DST-INSPIRE Camps for School students (as Mentor)
- Serving as liaison for Indo-German Cultural and Academic exchange programmes
- Jagadish Bose National Science Talent Search (JBNSTS) as Lecturer & Advisor
- R.K. Mission Institute of Culture (public lectures)
- Pedagogic lectures in different Colleges and Universities in India
- Lecturing in Summer Schools in IACS, KIIT and other institutes
- Refreshers' Courses for Physics Teachers in Calcutta Univ, Jadavpur University,
- C.K. Majumdar Memorial Workshop for B.Sc students, as resource person
- Lecturing in Condensed Matter Days
- Indian Science Congress, as plenary speaker and session coordinator

#### **12. SYMPOSIA, MEETING, SEMINARS AND SUMMER SCHOOLS ORGANIZED**

- Organizer of Theme Symposium “2D Materials beyond Graphene”, SMEC-2017 Conference, Miami, April 2017.
- Co-organizer of “Discussion Meeting on Nano-scale and Atomic-scale Quantum Structures and Devices”, IACS Kolkata, February 2016.
- Chairman of the Organizing Committee of “National Science Day – 2016”, IACS Kolkata, February 2016.
- Organizer (joint), Mini-Symposium on “New Energy Harvesting Materials Search by Computer Simulation”, in ICCP9 International Conference in Singapore, January 2015
- Co-organizer of “Multiscale Modeling of Materials and Devices” (MMMD-2014), Mumbai, November 2014.
- Organizer (from IACS) of the DWIH Program Excellence on Tour – 2014 programme of the German Research Foundation (DFG) March 2014.
- Organizer of Royal Society – DST Joint Scientific Seminar on “From Graphene Analogues to Topological Insulators” (GATI-2014), Vedic Village, January 2014.
- Chair, Theme Symposium on Computational Materials Science, IUMRS-ICA-2013, Bangalore, December 2013.

- Organizer (jointly with Prof. Rajeev Ahuja) of the symposium on "Hydrogen Storage, Production and Fuel Cells" at the SMEC-2013 Conference Miami, March 2013
- Coordinator of the C.V. Raman Symposium on Materials Science in the Centenary Session of Indian Science Congress.
- Chairman, Computational Materials Science Subject Group of the Materials Research Society of India (1999-present)
- Member of Executive Committee of the Asian Consortium for Computational Materials Science - ACCMS (2000 - present)
- Initiated national level Coordinated Research Project on Spintronics Materials (2006 – present)
- Member, DST-FIST Program Subject Expert Committee on Chemical Science (2008 - present)
- Heading the Materials Simulation Laboratory at IACS Kolkata (2005 – present)

### 13. PARTICIPATIONS IN INTERNATIONAL MEETINGS (not exhaustive list)

- *SMEC-2017 (Society for Materials under Extreme Conditions) Conference, Miami, April 2017* (Invited Talk)
- School of Photovoltaic & Renewable Energy Engineering (SPREE) Colloquium, UNSW, Sydney, Australia, November 2016 (Available on YouTube)
- IMURS-ICEM 2016 *Symposium-N* "Materials by Theoretical / Computational Design", Singapore, July 2016 (Invited Talk)
- 5th International Conference on Advances in Energy Research (ICAER 2015), IIT Bombay, December 2015 (Invited Talk).
- Conference on Computational Physics (CCP2015), IIT Guwahati, December 2015 (Invited Talk).
- International Conference on Recent Progress in Graphene and Two-dimensional Materials Research (RPGR-2015), Lorne, Victoria, October 2015 (Invited Talk).
- International Conference on Functional Materials for Frontier Energy Issues, Novosibirsk, Russia, October 2015 (Invited Talk).
- European Materials Research Society (E-MRS) Fall Meeting, Warsaw, September 2015 (Invited Talk).
- $\psi_k$ -2015 Conference on *Ab initio* (from the electronic structure) calculations of processes in materials, San Sebastian, September 2015.
- 8<sup>th</sup> Asian Conference on Computational Materials Science (ACCMS-8), Taipei, June 2015 (Invited Talk)
- 9<sup>th</sup> International Conference on Computational Physics (ICCP-9), NUS Singapore, January 2015 (Invited Talk).
- International Conference on Advanced Materials and Energy Technology (AMET-2014), IEST Shibpur, December 2014 (Key Note Lecture)
- First International Conference on Emerging Materials: Characterisation & Application (EMCA-2014), CGCRI Kolkata, (Plenary Lecture).
- Indo-US Workshop on Physics and Chemistry of Graphene and other single and bilayer materials including MoS<sub>2</sub> and phosphorene, IISc Bangalore, December 2014 (Invited Talk).
- 9<sup>th</sup> General Meeting of ACCMS-VO, OIST Okinawa, December 2014
- International Conference on Condensed Matter Physics (ICCMP-2014), Shimla, November 2014 (Invited Talk).
- International Symposium on Clusters, Cluster Assemblies and Nano-scale Materials (*ISCANM-III*), HRI Allahabad, March 2014 (Invited Talk).
- Physics of Surfaces and Interfaces (PSI-2014), Puri, February 2014 (Invited Talk).
- International Workshop on Nanotechnology and Applications (IWNA-2013), Vietnam, November 2013 (Invited Talk).
- 8<sup>th</sup> General Meeting of ACCMS-VO, Sendai, November 2013 (Invited Talk).

- 3<sup>rd</sup> International Conference on Advanced Nanoscience and Nanotechnology (ICANN-2013), IIT Guwahati, December 2013 (Invited Talk).
- IUMRS International Conference on Advanced Materials (ICAM), Qingdao, China, September 2013 (Invited Talk).
- 7<sup>th</sup> Conference of the Asian Consortium for Computational Materials Science (ACCMS-7), Thailand, July 2013 (Invited Talk).
- International Symposium on Recent Electronic Structure Theories and Related Experiments (ELSTRUC), Stuttgart, June 2013
- American Physics Society (APS) March Meeting, Baltimore, March 2013
- 7<sup>th</sup> Meeting of the Study of Matter at Extreme Conditions (SMEC), Miami, March 2013.
- International Symposium on Science of Clusters, Nanoparticles, and Nanoscale-Materials (SOCNAM), Jaipur, March 2013 (Invited Talk)
- 6<sup>th</sup> India-Singapore Joint Physics Symposium (ISJPS), IIT Kharagpur, February 2013 (Invited Talk).
- International Workshop on Computational Design of Materials for Energy Conversion and Storage, January 2013 (Invited Talk).
- 7<sup>th</sup> General Meeting of ACCMS-VO, Sendai, November 2012 (Invited Talk).
- IUMRS-ICEM 2012, Yokohama, September 2012 (Invited Talk).
- Asian Symposium on Hydrogen Storage (ASHM-2012), Jeju Island, S. Korea, April 2012 (Invited Talk)
- Summer School on Physics and Chemistry of Spintronics Materials, Orange County Coorg, February 2012 (Invited Talk).
- 6<sup>th</sup> General Meeting of ACCMS-VO, Sendai, February 2012 (Invited Talk).
- International Conference on Advanced Materials (ICAM-2011), PSG College of Technology, Coimbatore, December 2011 (Invited Talk)
- International Symposium on Clusters, Cluster Assemblies and Nano-scale Materials (ISCANM-II), HRI Allahabad, November 2011 (Invited Talk)
- “6<sup>th</sup> Conference of the Asian Consortium for Computational Materials Science (ACCMS-6), Singapore, September 2011 (Invited Talk).
- “1<sup>st</sup> Asian Symposium on Hydrogen Storage Materials”, Hanzhou, China, May 2011 (Invited talk).
- “4<sup>th</sup> India-Singapore Joint Physics Symposium”, NUS Singapore, February 2011 (Invited Talk)
- 5<sup>th</sup> General Conference of ACCMS-VO, IMR Sendai, December 2010 (Invited Talk)
- IUMRS-ICEM 2010, Seoul, Korea, August 2010 (Oral Presentation)
- Swedish-Asia Link Programme on Frontiers in Electronic Structure Calculations: Techniques and Applications, Pune University, February 2010 (Invited Talk).
- 4<sup>th</sup> General Meeting of ACCMS-VO, IMR Tohoku University, Sendai, January 2010 (Invited Talk).
- 5<sup>th</sup> Conference of the Asian Consortium for Computational Materials Science (ACCMS-5), Hanoi, Vietnam, September 2009 (Invited Talk).
- APCTP Conference on Recent Trends on Strongly Correlated Systems, IACS Kolkata, March 2009 (Invited Talk).
- 3<sup>rd</sup> General Meeting of ACCMS-VO, IMR Sendai February 2009 (Invited Talk)
- International Symposium on Clusters, Cluster Assemblies and Nanoscale Materials (ISCANM-2009), HRI Allahabad, February 2009 (Invited Talk)
- International Conference on Physics of Surfaces and Interfaces (PSI-2009), Toshali Sands, Puri, February 2009 (Invited Talk).
- Indo-US Workshop on Indo-US Workshop on Materials Design: Measurement, Modeling and Informatics, January, 2009 (Invited Talk).
- 11<sup>th</sup> International Symposium on Physics of Materials (ISPMA-11), Charles University, Prague, August 2008 (Invited Talk).

- Asia-Nano Conf, Symposium on Materials Issues in Hydrogen Storage, Singapore, July 2008 (Invited Talk)
- 2<sup>nd</sup> General Meeting of ACCMS-VO, IMR Sendai February 2008 (Invited Talk)
- India-Singapore Joint Symposium on Current Trends in Physics, IIT Madras, February 2008 (Invited Talk)
- 4<sup>th</sup> Conference of the Asian Consortium on Computational Materials Science (ACCMS-4), KIST Seoul, September 2007 (Invited Talk).
- EU-India Grid Training & Workshop on Materials, Earth & Atmospheric Sciences, Pune, September 2007 (Invited Talk).
- International Conference on Materials for Advanced Technology (ICMAT-2007), Singapore, July 2007 (Invited Talk).
- International Conference on Recent Trends in Many-body Methods for Electronic Structure & Properties of Atoms & Molecules, Toshali Sands, Puri, January 2007 (Invited Talk).
- Asia-Sweden Research Link Conference on Magnetism in Materials, Kolkata, January 2007 (Invited Talk).
- ACCMS Working Group Meeting on Clusters and Nanomaterials, Sendai, September 2006 (Invited Talk).
- International Conference on Advanced Materials Design & Development (ICAMMD-2005), Goa, December 2005 (Invited Talk).
- Third Conference of the Asian Consortium for Computational Materials Science (ACCMS-3), Beijing, China, September 2005 (*Invited Talk*)
- Second Conference of the Asian Consortium for Computational Materials Science (ACCMS-2), Novosibirsk, Russia, July 2004 (*Invited Talk*)
- Psi-k2000 Conference on ‘*Ab initio* calculation of complex processes in Materials’, SchwaebischGmuend, Germany, September, 2000.
- Indo-Japan Workshop on ‘Materials Design by Computer Simulation Sendai’, Japan, August 1999 (*Invited Talk*).
- Fifth IUMRS International Conference in Asia, Bangalore, India, 1998.
- International Symposium on ‘Novel Materials’, Bhubaneswar, India, 1997.
- Psi-k Network Conference on ‘*Ab initio* calculation of complex processes in materials’, Schwaebisch Gmuend, Germany, 1996.
- XX International Workshop on ‘Condensed Matter Theories (CMT-XX)’, Pune, India, 1996 (*Invited talk*).
- ICTP Working Group on ‘Disordered Alloys’, Trieste, Italy, 1994 (Lecture Course).
- International Conference on ‘Advances in Physical Metallurgy’ (ICPM-94), Bombay, India, 1994 (*Invited talk*).
- ICTP Workshop on ‘Methods of electronic structure calculations’, Trieste, Italy, 1992 (*Invited talk*).
- APS March Meeting, in St. Louis, USA, 1989 & in New Orleans, USA 1988.
- CECAM Workshop on ‘Electronic, Structural and Lattice-Dynamical Properties of semiconductor interfaces and superlattices’, Paris, France, 1988 (*Invited talk*).
- 18th International Conference on ‘Electronic structure of metals and alloys’, Dresden, Germany, 1988 (*Invited talk*).
- 8th International Conference on ‘Positron Annihilation’, Gent, Belgium, 1988.
- International School on ‘Electronic band structure and its applications’, Kanpur, India, 1986. (*Invited talk*).
- 7th International Conference on ‘Positron Annihilation’, New Delhi, India, 1985.



## 14. PUBLICATIONS

A. <i>Research Papers &amp; Review Articles</i> :	106 (101 International; 5 National)
B. <i>Articles published in edited volumes</i> :	17
C. <i>Book Chapters and Monographs</i> :	4
D. <i>Books/Volumes Edited</i> :	3
E. <i>International Conferences</i> :	50
F. <i>National Conferences</i> :	25+

\* *For details see List of Publications (enclosed).*

## 15. PROJECTS :

1. DMRL Project on Development of Computational Methodologies for Thermodynamics of Multicomponent Systems using Cluster Variation Method (2004-2006)  
*Target accomplished* : First-principles investigation of the electronic structure and bonding of different phases of Ti-Al and Ti-Al-Nb alloys
2. Coordinated Research Project on Spintronics Materials, Board of Research on Nuclear Sciences (BRNS) (2006-2010)  
*Target accomplished* : Electronic and Magnetic properties of 3d Transition Metal Doped II-VI DMO for nano-spintronics applications.
3. VR-SIDA Project on Hydrogen Storage Materials for Energy Applications (2012-15)  
*Target accomplished* : Computational design Li-functionalized hydrogenated nanosheet for H-storage
4. IACS-BARC Project on Quantum Structures and Phenomena (IBIQuS), (2009 - 2017) jointly with Prof. B.N. Dev, Dept of Materials Science, IACS (from Dept of Atomic Energy, under the 12<sup>th</sup> Five-year plan)  
*Target accomplished* : Design & Fabrication of quantum structures to explore fundamental science and device applications

## List of Publications (Dr. G.P. Das)

### A. Research Papers in Journals :

1. "First principles study of Ag absorption mechanism in amorphous large silica clusters", Sanchali Mitra, Rik Chattopadhyay, Mrinmay Pal, Gour Prasad Das, Shyamal Kumar Bhadra, *Physica E: Low-dimensional Systems and Nanostructures* (2019), DOI: [10.1016/j.physe.2019.03.013](https://doi.org/10.1016/j.physe.2019.03.013)
2. "Graphene wrapped organic nanotube: A promising material for ORR", M. Mukherjee, M. Samanta, S. Sarkar, **G.P. Das**, K.K. Chattopadhyay, *Materials Letters* (2019), DOI: [10.1016/j.matlet.2019.03.0132](https://doi.org/10.1016/j.matlet.2019.03.0132)
3. "Endorsement of Manganese Phthalocyanine microstructures as electrocatalyst in ORR: experimental and computational study", Moumita Mukherjee, M. Samanta, P. Banerjee, K. K Chattopadhyay, **G.P. Das**, *Electrochimica Acta* **296**, 528 (2019), DOI: [10.1016/j.electacta.2018.11.043](https://doi.org/10.1016/j.electacta.2018.11.043)
4. "TiS<sub>2</sub> Monolayer Emerging as Ultrathin Bifunctional Catalyst: Influence of Defect and Functionalization", Tisita Das, Sudip Chakraborty, Rajeev Ahuja and Gour P. Das, *Chem. Phys. Chem.* (2019), DOI: [10.1002/cphc.201801031](https://doi.org/10.1002/cphc.201801031)
5. "Origin of spin polarization in an edge boron doped zigzag graphene nanoribbon: a potential spin filter", Soubhik Chakrabarty, A H M Abdul Wasey, Ranjit Thapa and **G. P. Das**, *Nanotechnology* **29**, 345203 (2018)
6. "Tuning the electronic and magnetic properties of graphene/h-BN hetero nanoribbon: A first-principles investigation", Tisita Das, Soubhik Chakrabarty, Y. Kawazoe and **G. P. Das**, *AIP Advances* **8**, 65111 (2018)
7. "A new triazine based p-conjugated mesoporous 2D covalent organic framework: its in vitro anticancer activities", Sabuj K. Das, S. Mishra, K. Manna, U. Kayal, S. Mahapatra, K. Das Saha, S. Dalapati, G. P. Das, A.A. Mostafad and A. Bhaumik, *Chem. Commun.*, **54**, 11475 (2018).
8. "The origin of diverse lattice dynamics in the graphene family", Amrita Bhattacharya, P. R. Raghuvansi and **Gour P Das**, *J. Phys. Condens. Matt.* **30**, 355003 (2018).
9. "One pot solvothermal synthesis of ZnPc nanotube and its composite with RGO: A high performance ORR catalyst in alkaline medium", Moumita Mukherjee, M. Samanta, U.K. Ghorai, S. Murmu, **Gour P. Das**, Kalyan K. Chattopadhyay, *Appl. Surf. Sci.* **440**, 144 (2018).
10. "Electron doped C<sub>2</sub>N monolayer as efficient noble metal-free catalysts for CO oxidation", Soubhik Chakrabarty, Tisita Das, Paramita Banerjee, Ranjit Thapa, **G.P. Das**, *Appl. Surf. Sci.* **418**, 92 (2017),
11. "Exploring the catalytic activity of pristine T6[100] surface for oxygen reduction reaction: A first-principles study", Paramita Banerjee, Soubhik Chakrabarty, Ranjit Thapa and **G.P. Das**, *Appl. Surf. Sci.* **418**, 56 (2017).
12. "Graphene wrapped Copper Phthalocyanine nanotube: Enhanced photocatalytic activity for industrial waste water treatment", Moumita Mukherjee, U.K. Ghorai, M. Samanta, A. Santra, Gour P. Das, Kalyan K. Chattopadhyay, *Appl. Surf. Sci.* **418**, 156 (2017).
13. "Exploring adsorption and desorption characteristics of molecular hydrogen on neutral and charged Mg nanoclusters: A first principles study", Paramita Banerjee; K.R.S. Chandrakumar and **G. P. Das**, *Chem. Phys.* **469**, 123 (2016)
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