

## Prof. G.P. Das, Visiting Professor, Dept of Metallurgical & Materials Engg., IIT Kharagpur

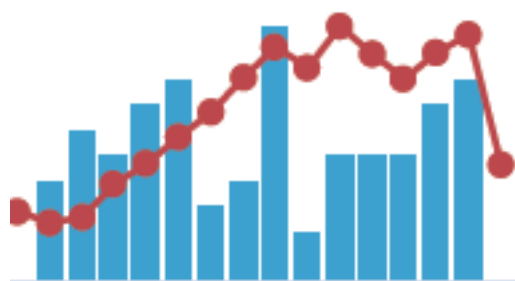
Prof. G.P. Das is a Computational Materials Scientist, who is well known for his contributions in the emerging field of materials modeling, simulation and design of alloys & intermetallics, interfaces & multilayers, clusters & nanostructures, etc. using density functional based first-principles techniques. During the past two decades, his research focus has been on spintronics materials, energy storage materials, functionalized 2D materials, and various kinds of quantum structures. After joining IIT Kharagpur in June 2018, Prof. Das has made significant contributions to both teaching and research, and has been instrumental in steering, guiding and advising students and young researchers in IITKgp. Within a rather short span of two years, he has interacted with several groups in IITKgp involved with materials science & engineering, who have fruitfully utilized his decades long experience, expertise as well as professional connectivity with other universities and research institutes, including several IITs in the country. Prof. Das has authored and co-authored ~150 papers, book chapters and review articles, (he has made ~15 peer reviewed publications during his 2-year tenure as Visiting Professor in IIT Kgp). He is a popular teacher and mentor, cutting across disciplines in basic sciences as well as engineering.

Prof. Das has 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 projects sponsored by DRDO, BRNS, JSPS etc., while more recently he has been involved with a multi-disciplinary project on Quantum Structures sponsored by the Department of Atomic Energy.

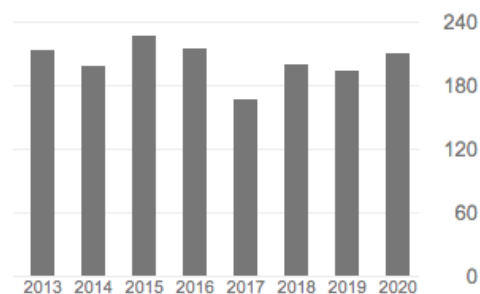
### 1. POSITIONS HELD

- 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
- Senior Scientist, Bhabha Atomic Research Centre, Mumbai, 1989-2004
- Scientific Officer, Bhabha Atomic Research Centre, Mumbai, 1978-1989
- Visiting Faculty Positions in Max Planck Institute for Solid State Research, Stuttgart (1987-89, 1992), Virginia Commonwealth University, Richmond (2001-02), Institute for Materials Research, Sendai (2010), University of New South Wales, Sydney (2016)
- Adjunct Professor, IEST Shibpur (2010), Distinguished Visiting Professor of PSG Institute of Advanced Studies, Coimbatore (2014), Adjunct Faculty, MAKAUT, WB (2019),

### 2. Publications (2019-20) : 11 peer reviewed journal articles, 2 popular articles, 3 Conference Proceedings, 1 Special issue of JPCM as Guest Editor [h-index 28, i-index 69, total citation ~3000]



Scopus



Google Scholar

### Journal Publications :

1. "Rapidly solidified Sm-Co-Hf-B magnetic Nano-composites: Experimental and DFT studies", A. Raja, T. Adhikary, I.A. Al-Omari, **G.P. Das**, S. Ghosh, D.K. Satapathy, A. Oraon, J.E. Shield, S. Aich, J. Magn. Mag. Mater. **504**, 166645 (2020).

2. "Probing mirror anomaly and classes of Dirac semimetals with circular dichroism". Abhirup Roy Karmakar, Snehasish Nandy, **Gour P. Das**, Kush Saha, arXiv:2004.14412 [cond-mat] (2020) [Under review in Physical Review Research]
3. "Reversible temperature dependent photoluminescence in a semiconductor quantum dot for development of smartphone-based optical thermometer", Partha Kumbhakar, Abhirup Roy Karmakar, **Gour P. Das**, Jayjeet Chakraborty, Chandra. S. Tiwary, Pathik Kumbhakar, Nanoscale Advances (2020), [under review]
4. "Vacancy Driven Tuning of Methane and Ammonia Decomposition on H- and T-phase TiS<sub>2</sub> Monolayer", Tisita Das, Sudip Chakraborty, Rajeev Ahuja, Yoshiyuki Kawazoe and **G.P. Das** [under 2<sup>nd</sup> round of review in Catalysis Today]
5. "Phonons and lattice thermal conductivities of graphene family", **Gour P. Das**, Parul R. Raghuvanshi and Amrita Bhattacharya, Procedia Structural Integrity **23**, 334 (2019)
6. "Investigation of ORR performances on graphene/Phthalocyanine nanocomposite in neutral medium", Moumita Mukherjee, M. Samanta, **Gour P. Das**, Kalyan K. Chattopadhyay, Microscopy & Microanalysis **25**, 1416 (2019)
7. "Functionalization and Defect-Driven Water Splitting Mechanism on a Quasi-Two-Dimensional TiO<sub>2</sub> Hexagonal Nanosheet", Tisita Das, Sudip Chakraborty, Rajeev Ahuja and **Gour P. Das**, ACS Appl. Energy Mater. **2**, 5074 (2019)
8. "First principles study of Ag absorption mechanism in amorphous large silica clusters", Sanchali Mitra, Rik Chattopadhyay, Shyamal Kumar Bhadra\_ Mrinmay Pal and **Gour P. Das**, Physica E : Low-dimensional Systems and Nanostructures **112**, 26 (2019)
9. "First-principles Identification of The Origin for Higher Activity of Surface Doped Carbon Nanohorn: Impact on Hydrogen Storage", Paramita Banerjee, Ranjit Thapa, A. Rajkamal, K.R.S. Chandrakumar and **G.P. Das**, Int. J. Hyd. Storage **44**, 23196 (2019)
10. "Graphene wrapped organic nanotube: A promising material for Oxygen Reduction Reaction", M. Mukherjee, M. Samanta, S. Sarkar, **Gour P. Das**, Kalyan K Chattopadhyay, Materials Letter **248**, 8-11 (2019).
11. "Endorsement of Manganese Phthalocyanine microstructures as electrocatalyst in ORR: experimental and computational study", Moumita Mukherjee, M. Samanta, P. Banerjee, K. K Chattopadhyay, **Gour P. Das**, *Electrochimica Acta* **296**, 528 (2019).
12. "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. **20**, 608 (2019).

#### Popular Level Articles :

1. "Renewable Energy and Hydrogen Economy", G.P. Das, SXC Physics Magazine *Horizon* (2020).
2. "Quantum Physics and Nanoscience", G.P. Das and M. Mukherjee, in '*Bahe Nirantara*' (2020), Magazine of Bethune College Physics Department to commemorate 50 years journey.

#### Contributed oral/poster presentations in conferences (from my group) :

- First principles investigation of Dirac semimetal ZrTe<sub>5</sub>, A.R. Karmakar, S. Nandy, **G.P. Das**, 2<sup>nd</sup> Indian Materials Conclave, Kolkata (February 2020)
- A survey in Deep-Reinforcement Learning for continuous control environments, Satya Prakash Dash, Sudeshna Sarkar and **G.P. Das**, ACCMS Theme Meeting, (2020) SRM-AP (January 2020)
- Exploring HER activity on zigzag graphene/h-BN hetero nanoribbon", Tisita Das and **Gour P. Das**, AIP Conf. Proc. **2115**, 30105 (2019)
- Quasi Two-Dimensional TiO<sub>2</sub> HNS Emerging as Efficient Catalyst for Hydrogen Generation, **Gour P. Das**, Tisita Das, Sudip Chakraborty, Rajeev Ahuja, Gordon Research Conference on Hydrogen-Metal Systems, Castelldefels, Spain (July 2019)
- Electronic and transport properties of graphene nanoribbon based prototype devices: first-principles study, **G.P. Das**, Soubhik Chakraborty, A.H.M. Abdul Wasey, Ranjit Thapa, 10th International Conference of ACCMS, Hong Kong (July 2019)

#### Invited Talks delivered in International Conferences :

- Invited talk in ACCMS-ICMG, SRM-AP (January, 2020)

- Invited talk in SCICON'19 Int. Conf, at Coimbatore (December 2019)
- Invited Talk in ICAM-2019 Int. Conf. at Kottayam (August 2019)
- Invited talk at ACCMS-10 at Hong Kong University (July 2019)
- Invited talk in EMAAT-2019, Shimla (June 2019)
- Keynote Lecture at MSMF-9 at Brno, Czech Republic (June 2019)
- Attended Gordon Conference on Hydrogen in Barcelona (June 2019)
- Invited Lecture ASM-2019 Workshop at IIT Delhi (*YouTube presentation*)
- Invited talk & session organizer in the 1<sup>st</sup> Indian Materials Conclave, Bangalore (February 2019)
- Invited talk in ICONN-2019, SRM Univ (January 2019)

### 3. List of activities

#### (a) Guiding Students (1 PhD, 1 MSc) :

- Currently Supervising one PhD Student Abhirup Roy Karmakar (18TS91R01, joined July 2018)  
Research Topic : "Theoretical Study of Topological Systems"
- One Integrated MSc Student Satya Prakash Dash (15PH20023) Master Thesis entitled "Continuous Control in Deep Reinforcement Learning and a Connection to Statistical Physics", submitted (2020)

#### (b) Teaching Courses (2019-20) :

- 2019-20 Spring Semester: CTS (TS66003) "*Micro-credit course on Time Dependent Density Functional Theory & its Applications*", Prof. D.G. Kanhere (CTS Coordinator: G.P. Das).
- 2019-20 Spring Semester: MME Dept (MT41028) : Atomistic Modelling of Materials
- 2019-20 Spring Semester: MME Dept (MT69002): Seminar for M.Tech,
- 2019-20 Spring Semester: Phys Dept (PH69008) : FMD Lab - II
- 2019-20 Autumn Semester: MME (MT41011) : Physics of Materials
- 2019-20 Autumn Semester: Phys. Dept (PH19001) : 1<sup>st</sup> Year Physics Lab
- Micro-credit course on "*First principles simulation of materials using density functional approach*", IIT Mandi, June 2019

#### (c) Research Collaborations & Miscellaneous Assignments at IIT Kharagpur :

- Collaboration with Prof. Shampa Aich, Dept of MME, on Materials for Permanent Magnets.
- Collaboration with Prof. Chandra Sekhar Tiwary, Dept of MME, on Functionalized 2D and other low dimensional materials.
- Acted as expert in the selection committee for recruitment of Assistant Professor in Materials Science Centre;
- Acted as member for scholar selection in Dept of Metallurgical & Materials Engg and in School of Nano-Science & Technology
- Conducted micro-credit course on Density Functional Theory at Centre for Theoretical Studies.
- External expert in PMRF Programme Committee at ISM Dhanbad (November 2019)
- Taken part in organizing Visit by German delegation to IIT Kharagpur (March 2019)

#### (d) Meetings organized :

- Psik-2020 Theme Symposium on "Materials for Energy" (as Chair): 14-17 September, 2020, postponed to September 2021 due to Covid-19 Pandemic.
- Webinar Series on "Materials Simulation: A Virtual Guided Tour", jointly organized by IIT Bombay, IIT Delhi, IIT Indore and IIT Kharagpur (May 2020)
- Theme Session on Computational Materials Science in 2<sup>nd</sup> Indian Materials Conclave, Kolkata (February, 2020)
- One-day Seminar on "Materials Simulation : from Classical to Quantum", IITKgp, May 2019
- One-day Symposium on "Applications of DFT and TDDFT in Materials and Molecules", in CTS (March, 2020)

#### 4. Honors and Accolades

- Guest Editor of a special issue "Ordering, Segregation and Order-Disorder Transition in Alloys" of the Journal of Physics: Condensed Matter, Vol. 32 (2020)  
<https://iopscience.iop.org/journal/0953-8984/page/Orderdisordertransitionalloys>
- Invited to chair Psik-2000 Theme Symposium on "Materials for Energy" in the Psik-2020, the largest world-wide network on electronic structure  
<https://www.psik2020.net/program/symposia>
- Adjunct Faculty, MAKAUT, WB (2019)
- Chairman of MRSI Subject Group on Computational Materials Science (continuing for 10 years)