

Name: Prof. Gour P. Das (GPD)

M.Sc., PhD

Department: Physics

Designation: Distinguished Visiting Faculty

Email ID: gpdas@sxccal.edu gourpdas@gmail.com

Research Field: Theoretical & Computational Condensed Matter Physics. Electronic, Magnetic & other ground state properties of materials from Bulk to Nano, Quantum structures, 2D Materials.



Academic Record :

- B.Sc. (Physics Hons), St. Xavier's College (1973)
- M.Sc. (Physics), Calcutta University (1975); Specialization in Solid State Physics
- Ph.D. (1986), Bombay University (1986); Dissertation *Electron Momentum Density Studies in Solids*

Positions held :

- Visiting Professor, IIT Kharagpur (June 2018 – June 2021)
- 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 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 Groningen, 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)

Awards and Distinctions

- 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)
- Recipient of Max Planck Fellowship (1987-89)

Meetings organized (only during the past two years) :

- Psik-2020 Theme Symposium on “Materials for Energy” (as Chair): 14-17 September, 2020, postponed to September 2021 due to Covid-19 Pandemic.
- Webinar on “Atomistic Modelling and Simulation of Materials”, IIT Kharagpur, 30-31 May, 2021
- 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 2nd Indian Materials Conclave, Kolkata (February, 2020)
- One-day Symposium on “Applications of DFT and TDDFT in Materials and Molecules”, in CTS (March, 2020).
- One-day Seminar on “Materials Simulation : from Classical to Quantum”, IITKgp, May 2019

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 :

- Advisory Editorial Board Member, Computational Condensed Matter, Elsevier (Since 2021)
- 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.

Membership of Professional bodies

- Life Member, Materials Research Society of India
- Life Member, Indian Physical Society.
- Life Member, Indian Physics Association
- Life Member, Asian Consortium for Computational Materials Science
- Member, American Physical Society

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 & 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, C.U. (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)

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
- ¶Subject-wise classification of papers available in 3-Volume Festschrift “*A Physicist’s Journey through the World of Materials*”, G.P. Das, (*Electronic Version available on request*)

Guiding Students :

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

Invited talks :

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

Major projects (As PI & Co-PI) :

- IACS-BARC Project on Quantum Structures and Phenomena (IBIQUS), (2009 - 2017) jointly with Prof. B.N. Dev, Dept of Materials Science, IACS (DAE Project under 12th Five-year plan)
- VR-SIDA Project on “Hydrogen Storage Materials for Energy Applications”, with Uppsala University, Sweden (2008-2012)
- Coordinated Research Project (CRP) 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)

Annexure

List of publications (during the last 10 years)

A. Research Papers in Journals :

1. "Probing mirror anomaly and classes of Dirac semimetals with circular dichroism". Abhirup Roy Karmakar, Snehasish Nandy, **Gour P. Das**, Kush Saha, Physical Review Research **3**, 013230 (2021).
2. "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 **13**, 2946 (2021).
3. "Charge transfer driven interaction of CH₄, CO₂ and NH₃ with TiS₂ monolayer: Influence of vacancy defect", Tisita Das, Sudip Chakraborty, Rajeev Ahuja, Y. Kawazoe, **Gour P. Das**, Catalysis Today **370**, 189 (2021).
4. "Computationally Exploring the Role of S-dopant and S-linker in Activating the Catalytic Efficiency of Graphene Quantum Dot for ORR", Paramita Banerjee, **G.P. Das** and Ranjit Thapa, Catalysis Today **370**, 36 (2021).
5. "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).
6. "Phonons and lattice thermal conductivities of graphene family", **Gour P. Das**, Parul R. Raghuvanshi and Amrita Bhattacharya, Procedia Structural Integrity **23**, 334 (2019)
7. "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)
8. "Functionalization and Defect-Driven Water Splitting Mechanism on a Quasi-Two-Dimensional TiO₂ Hexagonal Nanosheet", Tisita Das, Sudip Chakraborty, Rajeev Ahuja and **Gour P. Das**, ACS Appl. Energy Mater. **2**, 5074 (2019)
9. "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)
10. "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)
11. "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).
12. "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).
13. "TiS₂ 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).
14. "Origin of spin polarization in an edge boron doped zigzag graphene nanoribbon: a potential spin filter", Soubhik Chakraborty, A H M Abdul Wasey, Ranjit Thapa and **G. P. Das**, Nanotechnology **29**, 345203 (2018)
15. "Tuning the electronic and magnetic properties of graphene/h-BN hetero nanoribbon: A first principles investigation", Tisita Das, Soubhik Chakraborty, Y. Kawazoe and **G. P. Das**, AIP Advances **8**, 65111 (2018)

16. "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).
17. "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).
18. "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).
19. "Electron doped C₂N monolayer as efficient noble metal-free catalysts for CO oxidation", SoubhikChakrabarty, Tisita Das, Paramita Banerjee, RanjitThapa, **G. P. Das**, *Appl. Surf. Sci.* **418**, 92 (2017),
20. "Exploring the catalytic activity of pristine T6[100] surface for oxygen reduction reaction: A first principles study", Paramita Banerjee, SoubhikChakrabarty, RanjitThapa and **G. P. Das**, *Appl. Surf. Sci.* **418**, 56 (2017).
21. "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).
22. "Exploring the effect of oxygen coverage on the electronic, magnetic and chemical properties of Ni(111) supported h-BN sheet: A densityfunctional study", A.H.M. Abdul Wasey, **G.P. Das**, C. Majumder, *Chem. Phys. Lett.* **676**, 124 (2017).
23. "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)
24. "First principles design of Li functionalized hydrogenated h-BN nanosheet for hydrogen storage", Paramita Banerjee, BiswarupPathak, Rajeev Ahuja and **G.P. Das**, *Int. J. Hyd. Energy* **41**, 14437 (2016).
25. "Electronic Structure and Local Magnetism of 3d, 4d and 5d impurity substituted CeFe₂", Rakesh Das, **G. P. Das** and S.K. Srivastava, *J. Phys. D : Applied Physics* **49**, 165004 (2016).
26. "An extended fractal growth regime in the diffusion limited aggregation including edge diffusion", AritraGhosh, R. Batabyal, **G. P. Das** and B.N. Dev, *AIP Advances* **6**, 015301 (2016).
27. "First-principles Design of Divacancy Defected Graphene Nanoribbon based Rectifying and NDR Device", Soubhik Chakrabarty, A. H. M. Abdul Wasey, Ranjit Thapa and **G. P. Das**, *AIP Advances*, **5**, 087163 (2015).
28. Quantum size effects in layered VX₂ (X=S, Se) materials: Manifestation of metal to semimetal or semiconductor transition", A.H.M. Abdul Wasey, S. Chakrabarty, **G. P. Das**, *J. Appl. Phys.* **117**, 064313 (2015).
29. A first-principles study of III-IV-V semiconductor nanosheets", A. Bhattacharya, S. Bhattacharya, **G. P. Das**, *Phys. Chem. Chem. Phys.* **17**, 1039 (2015)
30. "Heteroepitaxial Junction in Au-ZnSe Nanostructure: Experiment versus First-principle Simulation", Riya Bose, A. H. M. Abdul Wasey, **G. P. Das** and Narayan Pradhan, *J. Phys. Chem. Lett.* **5**, 1892 (2014)
31. "Substrate induced modulation of electronic, magnetic and chemical properties of MoSe₂ monolayer", A.H.M. Abdul Wasey, Soubhik Chakrabarty and **G. P. Das**, *AIP Advances* **4**, 047107 (2014).
32. "Evolution of Fermi Level State Density in Ultrathin Films Near the Two-Dimensional Limit: Experiment and Theory", R. Batabyal, A. H. M. Abdul Wasey, J. C. Mahato, Debolina Das, **G. P. Das** and B. N. Dev, arXiv 1412.1238 [cond-mat.mtrl-sci] (2014).
33. "First principles density functional investigation of supported Tungsten cluster (W_n; n = 1 to 6) on anchored graphite (0001) surface", S. Barman and **G. P. Das**, *Int. J. Comp. Mater. Sci. Engg* **2**, 1350015(2013).

34. "h-BN monolayer on Ni(111) surface: A potential catalyst for oxidation", A.H.M. Abdul Wasey, S.Chakrabarty, **G. P. Das** and C. Majumder, *ACS Appl. Mater. Interfaces* **5**, 10404 (2013).
35. "Optical and vibrational properties of hydrogenated BN-sheet: First principles study", R. Thapa and **G. P. Das**, *Appl. Surface Sci.* **284**, 638 (2013).
36. "Exploring semiconductor substrates for Silicene epitaxy", A. Bhattacharya, S. Bhattacharya, **G.P. Das**, *Appl. Phys. Lett.* **103**, 123113 (2013).
37. "Manifestation of long-range ordered state in layered VX_2 [X=Cl, Br, I] systems", A.H.M. AbdulWasey, D. Karmakar and **G. P. Das**, *J. Phys. Condens. Matt.* **25**, 476001 (2013).
38. "Negative differential resistance in electron tunneling in ultrathin films near the two-dimensional limit", R. Batabyal, A.H.M. Abdul Wasey, J.C. Mahato, Debolina Das, A. Roy, **G. P. Das** and B.N. Dev, *J. Appl. Phys.* **113**, 34308 (2013).
39. "First principles electronic structure of coincidence site epitaxial Ag/Si(111) interface", A.H.M. Abdul Wasey, R. Batabyal, J.C. Mahato, B.N. Dev, Y. Kawazoe and **G. P. Das**, *Phys. Stat. Sol. B* **250**, 1313 (2012).
40. "Electronic structure of buried Co-Cu interface studied with photoemission spectroscopy", S. Banik, S. Barman, S.K. Rai, D.M. Phase, A.K. Srivastava, **G. P. Das** and S.K. Deb, *J. Appl. Phys.* **112**, 103702 (2012).
41. "Dehydrogenation Mechanism of Mono-ammoniated Lithium Amidoborane [Li(NH₃)NH₂BH₃]", S. Bhattacharya¹, ZhitaoXiong, Guotao Wu, Ping Chen, Y. P. Feng, C. Majumder, **G. P. Das**, *J. Phys. Chem C* **116**, 8859 (2012).
42. "Anti-Kubas type interaction in Hydrogen storage on a Li decorated BHNH sheet: A first-principles based study", S. Bhattacharya, A. Bhattacharya and **G. P. Das**, *J. Phys. Chem. C* **116**, 3840 (2012).
43. "Band gap engineering by functionalization of BN sheet", A. Bhattacharya, S. Bhattacharya and **G. P. Das**, *Phys. Rev. B* **85**, 035415 (2012).
44. "Strain induced band gap deformation of H/F passivated Graphene and h-BN sheet", A. Bhattacharya, S. Bhattacharya and **G. P. Das**, *Phys. Rev. B* **84**, 075454 (2011).
45. "Third conformer of graphene: A first-principles density functional theory study", A. Bhattacharya, S. Bhattacharya, C. Majumder and **G. P. Das**, *Phys. Rev. B* **83**, 033404 (2010).
46. "First-principles prediction of the third conformer of hydrogenated BN sheet", A. Bhattacharya, S. Bhattacharya, C. Majumder and **G. P. Das**, *Phys. Status Solidi RRL* **4**(12), 368 (2010).
47. "Magnetism in ZnO nanowire with Fe/Co codoping: First-principles density functional calculations", S. Ghosh, Q. Wang, **G. P. Das** and P. Jena, *Phys. Rev. B* **81**, 23215 (2010).
48. "Electronic structure and magnetic properties of (Fe,Co) codoped ZnO: Theory and Experiment", D. Karmakar, T.V. Chandrasekhar Rao, J.V. Yakhmi, A. Yaresko, V.N. Antonov, R.M. Kadam, S.K. Mandal, R. Adhikari, A.K. Das, T.K. Nath, N. Ganguli, I. Dasgupta and **G. P. Das**, *Phys. Rev. B* **81**, 184421 (2010)
49. "Effect of electron correlations on structural phase stability, magnetism, and spin-dependent transport in CeMnNi₄", M.S. Bahramy, P. Murugan, **G. P. Das** and Y. Kawazoe, *Phys. Rev. B* **81**, 165114 (2010).
50. "Transition metal decoration enhanced room temperature hydrogen storage in defect modulated graphene sheet", A. Bhattacharya, S. Bhattacharya, C. Majumder and **G. P. Das**, *J. Phys. Chem. C* **114**, 10297 (2010)
51. "Novel properties of boron nitride nanotubes encapsulated with Fe, Co, and Ni nanoclusters", S. Ghosh, S. Nigam, **G. P. Das** and C. Majumdar, *J. Chem. Phys.* **132**, 154704 (2010).
52. "Density functional calculations of hole induced long ranged ferromagnetic ordering in Mn doped Cd₂₈Se₂₈ nanocluster", S. Ghosh, B. Sanyal and **G. P. Das**, *Appl. Phys. Lett.* **96**, 52506 (2010); also reprinted in *Vir. J. Nan. Sci& Tech.* **21**(7) (2010).

53. Structural, electronic and magnetic properties of Cr-doped Cd₁₂S₁₂ clusters", S. Ghosh, B. Sanyal and **G. P. Das**, J. Magn. Mag. Mater. **322**, 734 (2010).
54. "3d transition metal decorated B-C-N composite nanostructures for efficient hydrogen storage: A first-principles study", S. Bhattacharya, C. Majumder and **G. P. Das**, Bull. Mater. Sci. **32**, 353 (2009); reprinted in the special issue of MRSI, C.N.R. Rao's 75th Birthday Volume, "Diversity in Materials Science", Ed. S.B Krupanidhi and H.K. Bhat, p.137 (2009).
55. "Ti-decorated BC₄N Sheet: A planar nanostructure for high-capacity hydrogen storage", S. Bhattacharya, C. Majumder and **G. P. Das**, J. Phys. Chem. C Lett. **113**, 15783 (2009).
56. "Enhanced magnetic moment in Fe-doped Pd_n clusters (n=1-13): a density functional study", S. Barman, D.G. Kanhere and **G. P. Das**, J. Phys.: Condens. Matter **21**, 396001 (2009).
57. "Pressure induced phase transition in tysonite LaF₃", P. Modak, A.K. Verma, S. Ghosh and **G. P. Das**, J. Phys. Chem. Sol. **70**, 922 (2009).
58. "Structural and electronic properties of Sn_{n-1}Pb and Pb_{n-1}Sn clusters: A theoretical investigation through first-principles calculations", S. Barman, C. Rajesh, **G. P. Das** and C. Majumdar, Eur. Phys. J. D **55**, 613 (2009).
59. "Electronic manifestation of cation-vacancy-induced magnetic moments in a transparent oxide semiconductor: Anatase Nb:TiO₂", S.X. Zhang, S.B. Ogale, W. Yu, X. Gao, T. Liu, S. Ghosh, **G. P. Das**, Andrew T.S. Wee, R.L. Greene and T. Venkatesan, Adv. Mater. **21**, 2282 (2009).
60. "Energetics and fragmentation of single-doped tin and lead clusters", B. Waldschmidt, S. Barman, C. Rajesh, C. Majumder, **G. P. Das** and R. Schaefer, Phys. Rev. B **79**, 045422 (2009).
61. "Hydrogen storage in Ti-decorated BC₄N nanotube", S. Bhattacharya, C. Majumder and **G. P. Das**, J. Phys. Chem. C (Letter) **112**, 17487 (2008)
62. "Ti decorated doped silicon fullerene: a possible hydrogen storage material", S. Barman, P. Sen and **G. P. Das**, J. Phys. Chem. C **112**, 19953 (2008)
63. "Lithium Calcium Imide (Li₂Ca(NH)₂] for hydrogen storage: Structural and Thermodynamics Properties", S. Bhattacharya, Gutao Wu, Chen Ping, Y.P. Feng and **G. P. Das**, J. Phys. Chem. B **112**, 11381 (2008)
64. "Electronic structure of GaN codoped with Mn and Cr", N. Tandon, **G. P. Das** and A. Kshirsagar, Phys. Rev. B **77**, 205206 (2008).
65. Co:CdS Diluted Magnetic Semiconductor Nanoparticles: Radiation Synthesis, Dopant-Defect Complex Formation and Unexpected Magnetism:, K.A. Bogle, S. Ghosh, S.D. Dhole, V.N. Bhoraskar, L.-F. Chi, N.D. Browning, D. Kundaliya, **G. P. Das** and S.B. Ogale, Chem Mater. **20**, 440 (2008)

B. Reviews Articles & Book Chapters :

66. "Simulation, Modeling and Design of Hydrogen Storage Materials", **G. P. Das** and Saswata Bhattacharya, Proc. Indian Natn. Sci. Acad. **81** (4), 939 (2015).
67. "First principles design of complex chemical hydrides as hydrogen storage materials", S. Bhattacharya and **G. P. Das**, in 'Concepts and Methods in Modern Theoretical Chemistry', Eds. S.K. Ghosh and P.K. Chattaraj (CRC Press, 2013), Chap.20, p.415.
68. "Spintronics: a revolution in materials science and semiconductor devices", **G. P. Das** and I. Dasgupta, Physics News, **38**, 46 (2008).

C. Edited volumes/proceedings :

69. "Ordering, Segregation and Order-Disorder Transition in Alloys", Guest Editors Sugata Mukherjee and **G.P. Das**, J. Phys. Condensed Matter Special Issue (2020)
70. Proceedings of the fifth conference of the Asian Consortium for Computational Materials Science (ACCMS-5), Eds. Duc Nguyen Manh, Yoshiyuki Kawazoe, **Gour Prasad Das** and

Nguyen Hong Quang, "Computational Materials Science", Vol. 49 Supplement 4, October 2010, Elsevier Publ.

D. Popular Articles :

71. "Renewable Energy and Hydrogen Economy", **G. P. Das**, SXC Physics Magazine *Horizon* (2020).
72. "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.

E. Articles published in symposia and conference volumes :

73. "Phonons and lattice thermal conductivities of graphene family", **Gour P. Das**, Parul R. Raghuvanshi and Amrita Bhattacharya, *Procedia Structural Integrity* **23**, 334 (2019)
74. "Valence band of Co/Cu thin film studied with synchrotronradiation photoemission spectroscopy", Soma Banik, S. K. Deb, S. Barman, **G. P. Das**, D. M. Phase and S. K. Rai, *Diamond Light Source Proceedings* **1**, e137 (2011).

F. Short Research papers :

75. "Cobalt Phthalocyanine (CoPc) Monolayer: A Computational Study on Oxygen Reduction Reaction (ORR)", M. Mukherjee, **G. P. Das** and Ayan Dutta, *AIP Conference Proceedings* **2265**, 030351 (2020); <https://doi.org/10.1063/5.0017060>
76. "Exploring HER Activity on Zigzag Graphene/h-BN HeteroNanoribbon", Tisita Das and **Gour P. Das**, *AIP Conference Proceedings* **2115**, 030105 (2019); <https://doi.org/10.1063/1.5112944>
77. "3d-Transition Metal Induced Enhancement Of Molecular Hydrogen Adsorption On Mg(0001) Surface: an *Ab-initio* Study", Paramita Banerjee and **G. P. Das**, *AIP Conf. Proc.* **1731**, 080028 (2016);
78. "Dehydrogenation Characteristics of $(\text{MgH}_2)_n$ ($n = 1-32$) Nanoclusters: A First-principles DFT study", P. Banerjee, K.R.S Chandrakumar and **G. P. Das**. *AIP Conf. Proc.* **1665**, 50065 (2015).
79. "Designing a new class of III-IV-V semiconductor nanosheets", A. Bhattacharya, S. Chakrabarty and **G. P. Das**, *AIP Conf. Proc.* **1512**, 850 (2013).
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81. "Frustrated non-collinearity in the magnetic behaviour of layered VX₂ [X=Cl, Br, I] systems", A.H.M. Abdul Wasey, D. Karmakar and **G. P. Das**, *AIP Conf. Proc.* **1512**, 1114 (2013)
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