# List of publications of G.P. Das since 2008

## *The complete list of publications has been compiled in 3-Volumes entitled "A Physicist's Journey through the World of Materials", G.P. Das, Vol 1-3 (2021)*

### *A. Research Papers in Journals :*

1. "Electronic and Magnetic Properties of Vanadium Dichalcogenides: A Brief Overview on Theory and Experiment". A.H.M. Abdul Wasey and **G. P. Das**, J. Appl. Phys. **131**, 190701 (2022).
2. "Manifestation of Interface-Induced Effects of Two-Dimensional MSi2/Si(111) Quantum Heterostructures: A First Principles Study", A.H.M. Abdul Wasey and **G.P. Das**, Physica E (2022), in press.
3. "Combined experimental and DFT studies of $Co_{82}Zr_{12}V_{6-x}B_x$ melt-spun ribbons to investigate structure and magnetic properties", A. Oraon, T. Adhikary, **G. P. Das**, S. Ghosh, A. Garg, A. Raja S. Aich, J. Magn. Mag. Mater. **547**, 168940 (2022).
4. "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).
5. "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, 13230 (2021).
6. "Charge transfer driven interaction of $CH_4$, $CO_2$ and $NH_3$ with $TiS_2$ monolayer: Influence of vacancy defect", Tisita Das, Sudip Chakrabarty, Rajeev Ahuja, Y. Kawazoe, **Gour P. Das**, Catalysis Today **370**, 189 (2021).
7. "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).
8. "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).
9. "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)
10. "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)
11. "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)
12. "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)
13. "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).
14. "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).
15. "$TiS_2$ 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).

16. "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)
17. "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)
18. "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).
19. "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).
20. "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).
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24. "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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26. "Electronic Structure and Local Magnetism of 3d, 4d and 5d impurity substituted $CeFe_2$", Rakesh Das, **G. P. Das** and S.K. Srivastava, J. Phys. D : Applied Physics 49, 165004 (2016).
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31. "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)
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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).
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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).
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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).
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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 $Cd_{12}S_{12}$ clusters", S. Ghosh, B. Sanyal and **G. P. Das**, J. Magn. Mag. Mater. **322**, 734 (2010).
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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:$TiO_2$", 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).
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64. "Electronic structure of GaN codoped with Mn and Cr", N. Tandon, **G. P. Das** and A. Kshirsagar, Phys. Rev. **B 77,** 205206 (2008).
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### *B. Reviews Articles :*

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. "Spintronics: a revolution in materials science and semiconductor devices", **G. P. Das** and I. Dasgupta, Physics News, **38**, 46 (2008).

### *C. Book Chapters :*

68. "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.

### *D. Edited volumes/proceedings :*

69. 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.

### *E. Articles published in symposia and conference volumes :*

70. "Renewable Energy and Hydrogen Economy", **G. P. Das**, SXC Physics Magazine *Horizon* (2020).
71. "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.
72. "Phonons and lattice thermal conductivities of graphene family", **Gour P. Das**, Parul R. Raghuvanshi and Amrita Bhattacharya, Procedia Structural Integrity **23**, 334 (2019)
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74. "Renewable Energy and Hydrogen Economy", **G. P. Das**, PANE Newsletter 1, 34 (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 Hetero Nanoribbon", 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);
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80. "Manifestation of surface and interface properties of Ag overlayer on Si(111)", A.H.M. Abdul Wasey, R. Batabyal, B.N. Dev and **G. P. Das**, AIP Conf. Proc. **1512**, 714 (2013)
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)
82. "Materials for Hydrogen Storage: From Complex Hydrides to Functionalized Nanostructures", **G. P. Das**, AIP Conf. Proc. **1349**, 58 (2010)
83. "Spintronic Materials: An Emerging Scenario", **G. P. Das**, Solid State Physics (India) **54**, 43 (2009), Proceedings of 54$^{th}$ DAE Solid State Physics Symposium.

### G. Manuscripts put up on arXiv and currently under review

84. "Magnetic Field Dependent Flexoelectricity in Atomically Thin $Co_2Te_3$", S. Demiss, A. Karstev, M. Palit, P. Pandey, **G. P. Das**, O.M. Femi, A.K. Roy, P. Kumbhakar, P. M. Ajayan, C.S. Tiwary, physics.app-ph arXiv: 2109.02781v1 (2021); and under review.
85. "Strain induced effects on the electronic and phononic properties of 2H and 1T' monolayer $MoS_2$", Saumen Chaudhuri, A. K. Das, **G. P. Das**, and B. N. Dev, cond-mat arXiv 2201.02174v1 (6 Jan 2022); and under review in Physica-B.
86. "Tensile Strain Induced Enhancement in Thermoelectric Performance of Monolayer $MoS_2$", Saumen Chaudhuri, A. Bhattacharya, A. K. Das, **G. P. Das** and B. N. Dev, cond-mat arXiv 2203.12991v1 (24 Mar 2022); and under review in 2D Materials.