

Publications from G.P. Das group: Materials for Energy Applications

[A] Hydrogen storage in complex light-metal hydrides

1. "Simulation, Modeling and Design of Hydrogen Storage Materials", G.P. Das and Saswata Bhattacharya, Proc. Indian National. Sci. Acad. **81** (4), 939 (2015).
2. "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
3. "Lithium Calcium Imide ($\text{Li}_2\text{Ca}(\text{NH})_2$) 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)
4. "Dehydrogenation Mechanism of Mono-ammoniated Lithium Amidoborane [$\text{Li}(\text{NH}_3)\text{NH}_2\text{BH}_3$]", S. Bhattacharya, Zhitao Xiong, Guotao Wu, Ping Chen, Y. P. Feng, C. Majumder, G.P. Das, J. Phys. Chem C **116**, 8859 (2012).

[B] Hydrogen storage in nano-clusters, nanosheets and nanohorns

5. "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).
6. "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).
7. "First principles design of Li functionalized hydrogenated h-BN nanosheet for hydrogen storage", Paramita Banerjee, Biswarup Pathak, Rajeev Ahuja and G.P. Das, Int. J. Hyd. Energy **41**, 14437 (2016).
8. "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).
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. "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)
11. "Hydrogen storage in Ti-decorated BC_4N nanotube", S. Bhattacharya, C. Majumder and G.P. Das, J. Phys. Chem. C (Letter) **112**, 17487 (2008)
12. "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).
13. "Ti-decorated BC_4N 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).

[C] Catalytic materials : Hydrogen Evolution and Oxygen Evolution Reactions

14. "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).

15. "Charge transfer driven interaction of CH₄, CO₂ and NH₃ with TiS₂ monolayer: Influence of vacancy defect", Tisita Das, Sudip Chakrabarty, Rajeev Ahuja, Y. Kawazoe, Gour P. Das, *Catalysis Today* **370**, 189 (2021).
16. "Functionalization and Defect-Driven Water Splitting Mechanism on a Quasi-Two-Dimensional TiO₂ Hexagonal Nanosheet", Tisita Das, Sudip Chakrabarty, Rajeev Ahuja and Gour P. Das, *ACS Appl. Energy Mater.* **2**, 5074 (2019).

[D] Electrocatalyst in Oxygen Reduction Reaction

17. "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).
18. "Graphene wrapped organic nanotube: A promising material for Oxygen Reduction Reaction", Moumita Mukherjee, M. Samanta, S. Sarkar, Gour P. Das, Kalyan K Chattopadhyay, *Materials Letter* **248**, 8-11 (2019).
19. "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).
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.* **449**, 144 (2018).
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. "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).
23. "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).

[E] Noble metal-free catalysts for CO oxidation

24. "Electron doped C₂N 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),
25. "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).

[F] Thermoelectric, Flexoelectric, Photoluminescent and other materials (manuscripts just appeared, in press, accepted and under review)

26. "Combined experimental and DFT studies of Co₈Zr₁₂V_{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).
27. "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 Chakrabarty, Chandra. S. Tiwary, Pathik Kumbhakar, *Nanoscale* **13**, 2946 (2021).

28. "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.
29. "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. (2022), in press.
30. "Magnetic Field Dependent Flexoelectricity in Atomically Thin Co₂Te₃", 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.
31. "Strain induced effects on the electronic and phononic properties of 2H and 1T' monolayer MoS₂", 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;
32. "Tensile Strain Induced Enhancement in Thermoelectric Performance of Monolayer MoS₂", 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;