

# List of Publications

## Related to Thesis

1. **B. R. Bhagat**, Alpa Dashora "Role of interlayer and interfacial electric field generated during simultaneous HER and OER over Li intercalated  $g - C_3N_4$  for efficient photocatalytic activity", Surfaces and Interfaces, 40, 103124 (2023).
2. **B.R. Bhagat**, Kishan H. Mali, Alpa Dashora "Surface activation of the  $g - C_3N_4$  by  $\pi$ -conjugation and interlayer orbital interaction to promote OER and HER", The Journal of Physical Chemistry C, 126 2573–2586 (2022).
3. **B.R. Bhagat**, Alpa Dashora "Understanding the synergistic effect of Co-loading and B-doping in  $g - C_3N_4$  for enhanced photocatalytic activity for overall solar water splitting", Carbon, 178 666-677 (2021).
4. **B.R. Bhagat**, Alpa Dashora Photocatalyst Potential Materials for Energy Production and Conversion", Energy Conversion and Green Energy Storage, CRC Press 3-28 (2022)
5. **B.R. Bhagat**, Alpa Dashora "Charge transfer mediated hydrogen evolution reaction of Co loaded  $g - C_3N_4$ ", Proceedings of the 65th DAE Solid State Physics Symposium (2021).

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## Other than Thesis

1. Avani Chunduri, Aniruddha Bhide, Suraj Gupta, Kishan H. Mali, **B. R. Bhagat**, Alpa Dashora, Matjaž Spreitzer, Rohan Fernandes, Rupali Patel, and Nainesh Patel "[Exploring the Role of Multi-Catalytic Sites in an Amorphous Co–W–B Electrocatalyst for Hydrogen and Oxygen Evolution Reactions](#)", ACS Applied Energy Materials, 6, 9, 4630–4641 (2023).
2. H.S. Mund, Kishan H. Mali, Kishor Kumar, Shailja Tiwari, **B.R. Bhagat**, Y. Sakurai, H. Sakurai, Alpa Dashora, B.L. Ahuja "[Understanding the effect of Ni and Co doping in magnetic properties of  \$La\_{0.7}Ca\_{0.3}MnO\_3\$ : Magnetic Compton spectroscopy and DFT strategies](#)", Journal of Magnetism and Magnetic Materials, 565, 170255 (2023).
3. Soumalya Kundu, Rahul Majumder, **B.R. Bhagat**, Subhadip Roy, Rabindranath Gayen, Alpa Dashora, Manish Pal Chowdhury "[An in situ synthesis of polyaniline/reduced graphene oxide nanocomposite flexible thin film on PET for the room temperature detection of trace level ammonia at ppb level](#)", Journal of Materials Science, 58, 3147 (2023).
4. Aditi Gaur, **B.R. Bhagat**, Jagrati Sahariya, Amit Soni, Alpa Dashora "[Design and study of  \$SrSnX\_2\$  \(X=N, P, Sb, As, Bi\) semiconductors using density functional theory](#)", Optik, 270, 170088 (2022).
5. Rahul K. Choudhury, **B.R. Bhagat**, Kishan H. Mali, Rushikesh Pokar, Alpa Dashora "[Effect of surface functional group over tungsten carbide MXene for efficient  \$NH\_3\$  gas sensing using density functional theory](#)", Applied Surface Science, 603, 154426 (2022).
6. A. Yadav, S. Gupta, **B.R. Bhagat**, M. Yadav, Alpa Dashora, R.S. Varma, N. Thorat, R. Patel, N. Patel "[Unraveling the synergy between oxygen doping and embedding Fe nanoparticles in  \$gC\_3N\_4\$  towards enhanced photocatalytic rates](#)", Applied Surface Science, 603, 154404 (2022).

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7. Aditi Gaur, Karina Khan, **B.R. Bhagat**, J. Sahariya, A. Soni, Alpa Dashora "Role of intermediate band and carrier mobility in Sn and Fe-doped  $CuAlS_2$  thin film for solar cell: A computational modelling", Solar Energy, 215 144-150 (2021).
  8. M. Saleem, **B.R. Bhagat**, A. Mishra "Influence of Lead Free  $Bi_{0.5}Na_{0.5}TiO_3$  Substitution on the Structural and Electrical Properties of Ferromagnetic Metallic Phase  $La_{0.8}Sr_{0.2}MnO_3$ ", Journal of Inorganic and Organometallic Polymers and Materials, Springer 29(6) 2103-15 (2019).
  9. **B.R. Bhagat**, Rushikesh Pokar, Alpa Dashora "First Principles Study of Novel  $BaSn_{1-x}In_xN_2$  (X=0, 0.25) for Thermoelectric Applications", Intelligent Computing Techniques for Smart Energy Systems. Lecture Notes in Electrical Engineering, 862 463–472 (2022)
  10. Kishan H. Mali **B.R. Bhagat**, Alpa Dashora "Ab-Initio Investigation of Electronic and Magnetic Properties of 2D Mn Doped  $Mo_2NT_2$  (T: O/F)", Intelligent Computing Techniques for Smart Energy Systems. Lecture Notes in Electrical Engineering, 862 553–563 (2022).
  11. Kishan H. Mali, **B.R. Bhagat**, Alpa Dashora "Tailoring electronic property of bilayer tri-s-triazine using spatial modification: An *ab initio* Study", Journal of Physics: Conference Series, 1849(1) 012028 (2021).
  12. Athira K.M., **B.R. Bhagat**, Alpa Dashora "Tuning of Electronic and Magnetic Properties in 2D van der Waals Hybrid Ferromagnet ( $Fe_3GeTe_2/Co_3GeTe_2$ )", AIP Conference Proceedings, 2369, 020079 (2021).
  13. M. Saleem, N. Bajpai, **B. Bhaghat**, M. Soni, M. Varshney, A. Mishra and D. Varshney "Studies on composites of homo-structured  $La_{0.8}Sr_{0.2}MnO_3$  and  $Bi_{0.5}Na_{0.5}TiO_3$ : Synthesis, structure and dielectric properties", AIP Conference Proceedings 2142(1) 040001 (2019)

## List of Presentations

1. Participated and presented a poster in VII – Rajasthan Science Congress-2019, Mohanlal Sukhadia University, Gujarat on “Enhancing photocatalytic behavior of ZnS: A Computational Perspective”, won the Prof. R. S. Paroda Best Presentation Award
2. Participated and gave an oral presentation at the National Research Scholars’ Meet on Condensed Matter Physics and Materials Science-2023, Gujarat University, Gujarat on “Possible CO<sub>2</sub> reduction pathways on the single-atom catalyst (Co–g–C<sub>3</sub>N<sub>4</sub>)”, won the Best Oral Presentation Award
3. Bestowed Young Scientist Award at the 2nd National Conference on Inter- disciplinary Approaches in Environmental Sciences-2023, The M. S. University of Baroda, Gujarat on “Single Atom vs Cluster Decorated Catalyst (Co–gCN/Co<sub>4</sub>B<sub>4</sub>–gCN): Guiding CO<sub>2</sub> Reduction Mechanism”, with a cash prize of Rs. 5000
4. Participated and gave a poster presentation at the National Conference on Scientific Innovations towards Developed India-2024, The M. S. University of Baroda, Gujarat on “Schottky Barrier to Ohmic Contact: Investigating Dimensionality of co-catalyst over g–C<sub>3</sub>N<sub>4</sub>”, won the Best Poster Presentation Award
5. Participated and gave an oral presentation at IX International Conference on Perspectives in Vibration Spectroscopy (ICOPVS), UGC-DAE Consortium for Scientific Research and Devi Ahilya Vishwavidyalaya, 2022
6. Participated and gave an oral presentation at the International Conference on Advances in Chemical and Materials Sciences (ACMS), Heritage Institute of Technology, 2022.
7. Participated and presented a poster in Ab-initio Many-Body Methods and Simulations with the Yambo Code, The Abdus Salam International Centre for Theoretical Physics, 2022.
8. Participated and gave an oral presentation on Intelligent Techniques for smart energy systems (ICTSES), Manipal University, 2021.
9. Participated and presented a poster in the 20th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, The Abdus Salam International Centre for Theoretical Physics, 2021.
10. Participated and presented a poster at the International Winter School on frontiers in materials science, Jawaharlal Nehru Centre for Advanced Scientific Research, 2020.

11. Participated and presented a poster in an Online workshop on Excited Charge Dynamics in Semiconductors, The Abdus Salam International Centre for Theoretical Physics, 2020.
12. Participated, and presented the paper at International Conference on Nano Science and Technology, S. N. Bose National Centre for Basic Sciences, 2020.