

Curriculum Vitae of

Ms. Baraiya Bhumi Arunkumar

Department of Physics,

Faculty of Science, The M. S. University of Baroda,

Vadodara – 390002. Gujarat, India

Present Designation: Senior Research Fellow (DST-INSPIRE),
The M. S. University of Baroda (2019 – Till date)

Title of the Thesis: Density Functional Theory of Free and Oxide Supported Metal Nanoclusters and Nanoalloys: A Heterogeneous Catalysis

Ph.D. Supervisor: Prof. Prafulla Kumar Jha

Personal Details

Address for Correspondence: Department of Physics, Faculty of Science,
The M. S. University of Baroda, Vadodara – 390002, Gujarat, India

Residential Address: Plot No – 562, Juni Vitthalvadi, Bhavnagar – 364001,
Gujarat, India

Sex: Female

Date of Birth: 13th January 1991

Nationality: Indian

Marital status: Unmarried

Passport Number: R0013525

Mobile no: 9824795279

Email: bhumiibaraiya@gmail.com

Native Language: Gujarati

Proficiency in Language: Gujarati, Hindi, English

Education and Academic Qualifications

- **Gujarat State Eligibility Test (GSET):** 2017
[Qualified in Physics]: Gujarat SET Agency, The M. S. University of Baroda, Vadodara, (Accredited by UGC, New Delhi)

- **Junior Research Fellow:** 2016 – 2019
[DST-INSPIRE]: Department of Physics, The M. S. University of Baroda

- **M. Sc. (Physics):** 2012 - 2014
[Gold Medalist]: Department of Physics, Faculty of Science, M. K. Bhavnagar University, Bhavnagar – 3640002, Gujarat, India

- **B. Sc. (Physics):** 2009 - 2012
[Distinction]: Sir P. P. Institute of Science, Bhavnagar – 364002, Gujarat, India.

- **12th Class (GSHEB):** 2008
[Second Class]: St. Xavier's Higher Secondary School, Bhavnagar

- **10th Class (GSHEB):** 2006
[Distinction]: Shree M. K. Jamod High School, Bhavnagar

Teaching Experience

- Teaching Assistant (PG Level), Department of Physics, M. K. Bhavnagar University, Bhavnagar – 364002, Gujarat, India. (August 2015 – May 2016).

Academic Awards/Prize/Fellowship

Sr. No	Name of Award	Awarding Agency	Year
1.	International Travel Support	Science and Engineering Research Board, DST, Govt. of India	2019
2.	Senior Research Fellow (Inspire Fellowship)	Department of science and technology (DST), Govt. of India	2019
3.	Student Travel Award Participate in “6 th Nano Today conference”	Elsevier	2018
4.	Junior Research Fellow (Inspire Fellowship)	Department of science and technology (DST), Govt. of India	2016
5.	LT. Shri Dr. Rohit Bhatt GOLD MEDAL	M. K. Bhavnagar University	2016
6.	Dr. R. V. Mehta Prize	M. K. Bhavnagar University	2016

Broad Subject area: Condensed Matter and Materials Physics, Density Functional Theory, Nanomaterials.

Specific Area of Research Interest

To investigate the atomic and electronic structure of free and oxide supported nanoclusters and nanoalloys to understand their morphology and bonding configurations, behavior at the molecular level, modified electronic and dynamical properties and optical transitions in adsorbed systems using Density Functional Theory (DFT) calculations.

Conference/Visit to abroad/School/Workshop Attended

- Doping effect on the Adsorption and Dissociation of CO₂ over Cage like Co₁₂M Bimetallic clusters (Oral presentation on ONLINE Mode) **National Conference on Recent Advancements in Materials science And Nanotechnology (RAMAN)-2020**, Nirma University, Ahmedabad, Gujarat. (July 30 - August 01, 2020)
(Achieve 2nd Rank in Oral Presentation)
- Scrupulous Detection of Poisonous Carbon Monoxide over Core-shell Pt_xMY (Where X + Y = 13) Nanoclusters: A Surface-Enhanced Raman Spectroscopy Study at **VIII International Conference on Perspectives in Vibrational Spectroscopy**, JNCASR, Bangalore, Karnataka, India. (24th - 29th, Feb 2020)
- **Poland Visit: (28th Jan to 6th February 2020)**
Title: “Role of Metal Surfaces in Heterogeneous Catalysis” (Orally Presented)
 - Materials Design Division, Faculty of Materials Science and Engineering, Warsaw University of Technology, 141 Wołoska Str., 02-507 Warsaw, Poland.
 - Faculty of Mechanical Engineering, Bialystok University of Technology, 45C Wiejska Str., 15-351, Bialystok, Poland.
- Adsorption of CO over Cu_nPd Bimetallic Clusters: A First-Principles Calculations at **Second International School on Nanoalloys (ISNA-2)**, Pisa, Italy. (20th - 27th January 2020)
(International Travel Support – ITS, SERB, Govt. of India, Oral and Poster Presented)

- Degrading CO Poisoning over Foreign Atom Seized Ag_{12}M Icosahedral Bimetallic Clusters at **64th DAE Solid State Physics Symposium**, IIT Jodhpur, Jodhpur, Rajasthan, India. (18th - 22nd Dec 2019)

- The Role of Doping on the Adsorption and Dissociation of CO_2 on Icosahedral Co_{12}M Bimetallic clusters at **The First-DAE Computational Chemistry Symposium (DAE-CCS 2019)** at BARC Mumbai, India. (7th - 9th Nov 2019)

- Density Functional Theory of Free and Oxide Supported Metal Nanoclusters and Nanoalloys: A Heterogeneous Catalysis at Attended and Presented Research Work at the **Inspire Review Meet**. (26th July 2019)

- O-assisted and pristine Au-Pt(100) surfaces: A platform for adsorption and decomposition of H_2O at **Indo-German Bilateral Workshop on Membranes for Water and Energy**, CSIR-Central Salt and Marine Chemicals Research Institute, Bhavnagar, Gujarat, India. (18th - 20th Feb 2019)

- *Interaction Mechanism of CO with Pd-Rich Copper Clusters* at **63rd DAE Solid State Physics Symposium**, Guru Jambheshwar University of Science and Technology, Hisar, Haryana, India. (18th - 22nd Dec 2018)

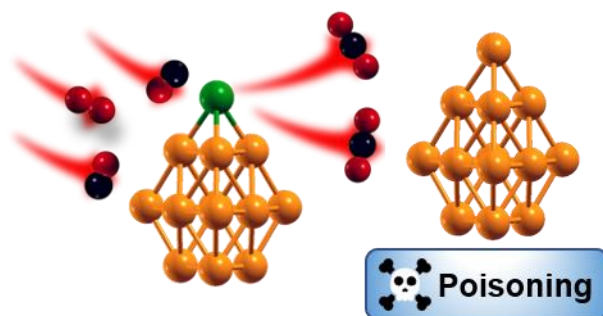
- *Nitrogen Decorated Borophene: An Empowering Contestant for Hydrogen Storage* at **International Conference on Materials for Energy Applications**, S.S. Jain Subodh P.G. (Autonomous) College, Jaipur, Rajasthan, India. (Oral Presentation) (6th - 8th Dec 2018)

- Vibrational Dynamics of CO Adsorbed Cu_{n+1} and Cu_nPd , Clusters at 7th **International Conference on Perspectives in Vibrational Spectroscopy**, BARC, Mumbai, India. (25th - 29th Nov, 2018)
- Investigation of CO Adsorption on the Cu_{n+1} and Cu_nPd Clusters at **National Conference on Advance in Spectroscopy: Molecules to Materials**, IIT-RAM, Ahmedabad, Gujarat, India. (4th - 6th Oct 2018)
- Adsorption Energetics of Nitric Oxides on Pt(111) Surface: A First Principles Investigation with DFT-D2 Correction at **International Conference on Nano-materials for Energy Conversion and Storage Applications**, PDPU, Gandhinagar, Gujarat, India. (29th - 31st Jan 2018)
- A First Principles Study of the Adsorption of C_2 , N_2 and S_2 Gases on Pt(111) Surface: General Trends at **National Conference on Recent Trends in Condensed Matter Physics**, Kolkata, West Bengal, India. (31st Oct - 3rd Nov 2018)
- Vibrational properties of III-V semiconductor in wurtzite phase: A comparative density functional theory study at **61st DAE-Solid State Physics Symposium** at KIIT University, Bhubaneswar, Odisha, India. (26th - 30th Dec 2016)
- IUCAA workshop on Electromagnetic scattering as a tool in Astronomy and Astrophysics, M. K. Bhavnagar University, Bhavnagar, Gujarat, India. (Attended). (4th - 5th Jan 2016)

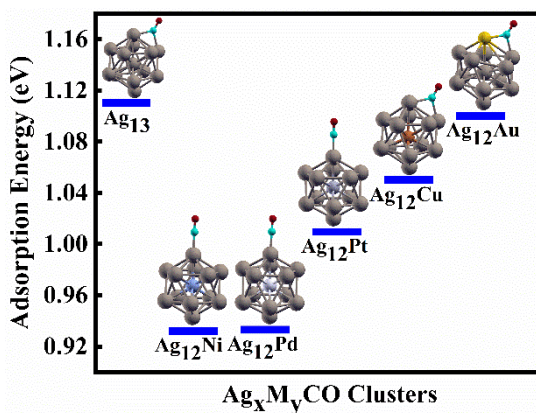
- National Conference on Recent Trends in Science of Materials at the The M. S. University of Baroda, Vadodara. (Attended) (28th - 30th Dec 2015)
- National level science symposium in Christ college at Rajkot in 2013. (Attended).

Publications

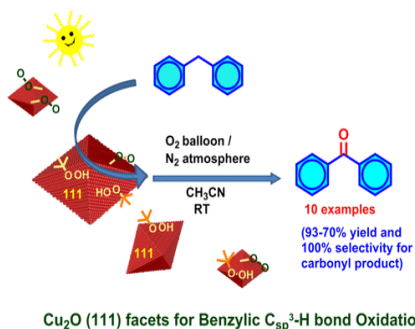
14. Bhumi A. Baraiya, Hemang Tanna, Venu Mankad, and Prafulla K. Jha, Dressing of Cu Atom over Nickel Cluster Stimulating the Poisoning-Free CO Oxidation: An Ab Initio Study, *The Journal of Physical Chemistry A*, 125, 5256-5272, (2021). DOI: /10.1021/acs.jpca.1c02354.



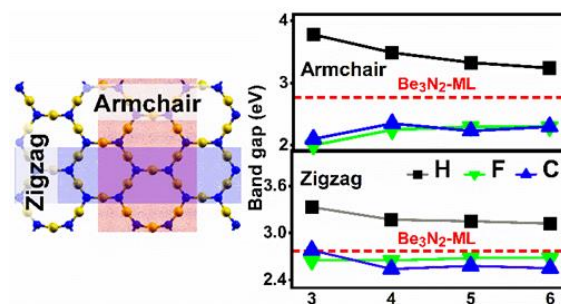
13. Bhumi A. Baraiya, Venu Mankad, Prafulla K Jha, Degrading CO poisoning over foreign atom seized Ag₁₂M icosahedral bimetallic clusters, *AIP Conference Proceedings*, 2265, 030612, (2020). DOI: 10.1063/5.0016620.



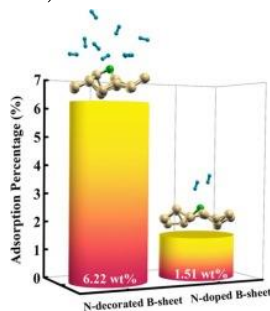
12. Neelam Gupta, Hiren K. Machhi, **Bhumi A. Baraiya**, Saurabh S. Soni, Ashutosh V. Bedekar, Prafulla K. Jha, and Hemant P. Soni, Benzylic C_{sp}³-H Bond Oxidation on the (111) Facets of Octahedral Cu₂O Nanocrystals, [ACS Applied Nano Materials](#), **Article ASAP**, (2021). DOI: 10.1021/acsanm.1c01169.



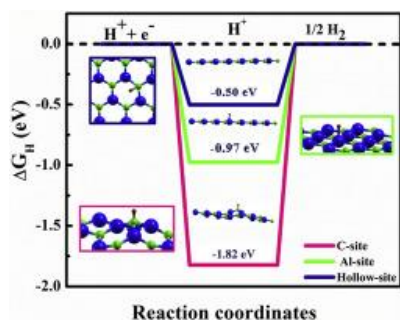
11. Aditya Dey, **Bhumi A. Baraiya**, Souren Adhikary, Prafulla K. Jha, First-Principles Calculations of the Effects of Edge Functionalization and Size on the Band Gap of Be₃N₂ Nanoribbons: Implications for Nanoelectronic Devices, [ACS Applied Nano Materials](#), **4**, 493-502, 2020. DOI: 10.1021/acsanm.0c02809.



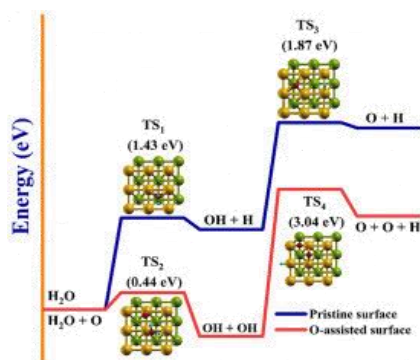
10. **Bhumi A. Baraiya**, Narayan N Som, Venu Mankad, Guangfen Wu, Jinlan Wang and Prafulla K. Jha, Nitrogen-Decorated Borophene: An Empowering Contestant for Hydrogen Storage, [Applied Surface Science](#), **527**, 146852, (2020). DOI: 10.1016/j.apsusc.2020.146852.



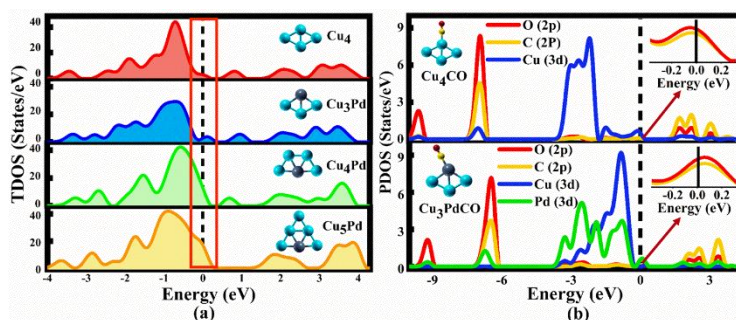
6. Khushbu Patel, **Bhumi A. Baraiya**, Narayan N. Som, Basant Roondhe, Prafulla K. Jha, Investigating Newly Predicted Honeycomb 2D h-AlC for Hydrogen Evolution Reaction: A DFT study, [International Journal of Hydrogen Energy](#), **45**, 18602-18611, (2019). DOI: 10.1016/j.ijhydene.2019.10.131.



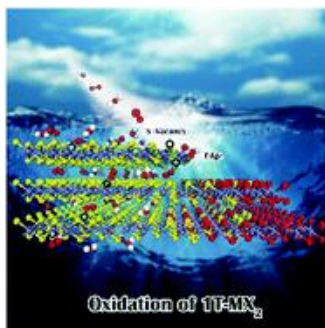
5. **Bhumi A. Baraiya**, Venu Mankad, Piotr Śpiewak, Krzysztof J Kurzydłowski, Prafulla K. jha, O-assisted and pristine Au-Pt(100) surfaces: A platform for adsorption and decomposition of H₂O, [International Journal of Hydrogen Energy](#) **45**, 18666-18675, (2020). DOI: 10.1016/j.ijhydene.2019.06.201.



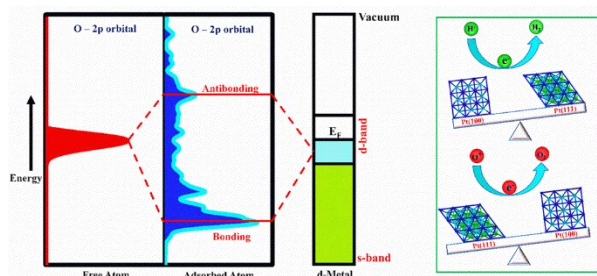
4. **Bhumi A. Baraiya**, Venu Mankad and Prafulla K. Jha, Interaction Mechanism of CO with Pd-Rich Copper Clusters, [AIP Conference Proceedings](#), **2115**, 030543 (2019). DOI: 10.1063/1.5113382.



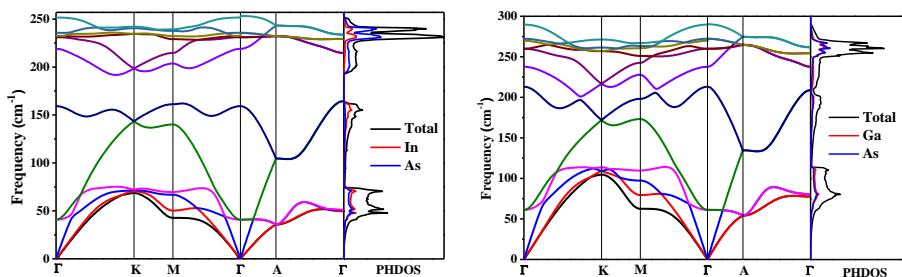
3. Qiang Li, Li Shi, Ruchun Wu, Chongyi Lin, Xiaowan Bai, Yixin Ouyang, **Bhumi A. Baraiya**, Prafulla K. Jha and Jinlan Wang, Unveiling chemical reactivity and oxidation of 1T-phased group VI disulfides, [Physical Chemistry Chemical Physics](#), **21**, 17010-17017 (2019). DOI: 10.1039/C9CP02985K.



2. **Bhumi A. Baraiya**, Venu Mankad and Prafulla K. Jha, Adsorption Energetics of Atoms and Diatomic Gases with Electrocatalysis Approach towards Hydrogen and Oxygen Evolution Reaction on Pt Surfaces, [ChemistrySelect](#), **3**, 10515–1052 (2018). DOI: 10.1002/slct.201802072.



1. Trupti K. Gajaria, Shweta D. Dabhi, **Bhumi A. Baraiya**, Venu Mankad and Prafulla K. Jha, Vibrational properties of III-V Semiconductor in Wurtzite Phase: A Comparative Density Functional Theory Study, [AIP Conference Proceedings](#), **1832**, 090043, (2017). DOI: 10.1063/1.4980596.



Skills and Expertise

- ✧ Operating Systems like DOS, CentOS, Linux, Windows XP/8/10,
- ✧ Simulation Packages like Quantum Espresso, VASP, Gaussian09, ATK-VNL, FDMNES, MKMKXX (microkinetic modelling)
- ✧ Plotting Packages like GNUplot, Xmgrace, Origin Pro
- ✧ Visualization Software like XCrySDen, Vesta, GaussView, VMD etc.

References

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