Shweta D. Dabhi

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Date of Birth: 1st January 1990
Nationality: Indian

EDUCATIONAL DETAILS

- Ph. D. (Physics) 2012-2017
  Title: Electronic and Vibrational Properties of Hybrid Nanostructures
  Ph.D. Supervisor : Prof. Prafulla Kumar Jha
- M. Sc. (Physics) [Gold Medalist] 2010-2012
  First Class with Distinction M. K. Bhavnagar University
- B. Sc. (Physics) 2007-2010
  First Class; Bhavnagar University
- Higher Secondary Class: Gujarat State Education Board 2005-2007
  First Class with Distinction
- Secondary Class: Gujarat State Education Board 2002-2005
  First Class with Distinction

ACADAMIC ACHIEVEMENTS

- ***BEST POSTER Award*** in "Recent Trends in Condensed Matter Physics" at Bose Institute, Kolkata. (2017).
- Awarded ***BEST ORAL PRESENTATION*** in "National Conference on Recent Trends in Science of Materials" at The M. S. University of Baroda (Dec 2015).
- Awarded ***Student Travel Award*** to participate in "4th NANO TODAY Conference" at Dubai, Organized by **Elsevier** (Dec 2015).

- Selected for ***DST-International Travel Support*** to present a paper in international conference at Germany (Sept 2015).
- Awarded DST-INSPIRE ***Senior Research Fellowship*** (Jan 2015-Dec 2017)
- ***BEST POSTER AWARD*** in 59th DAE Solid State Physics Symposium at VIT University, Vellore (Dec 2014).
- ***FIRST PRIZE FOR ORAL PRESENTATION*** in SERB School on "Density Functional Theory and Beyond" at The M. S. University of Baroda (2014).
- Awarded ***GOLD MEDAL*** and for the highest marks in M.Sc. Physics (2014).
- Qualified ***UGC-CSIR NET*** with All India Rank 123 (Dec. 2012). Other national level examination: ***GATE*** (2013), ***JEST*** (2012) and ***GSLET*** (2013).
- ***Minaxi Lalit Science Award*** by Gujarat Science Academy (2008, '09, '12).
- ***INSPIRE FELLOWSHIP Research Award*** by Department of Science and Technology, New Delhi (2012).
- For the First Rank in center in H.S.C. Examination, awarded "Kanya Kelwani Nidhi" prize from Govt. of Gujarat (2007).

LIST OF PUBLICATIONS

1. Trupti K. Gajaria, Basant Roondhe, Shweta D. Dabhi, and P. K. Jha "Exploring the Hidden Catalyst from Boron Pnictide Family for HER and OER", Accepted, *Int. J. Hydrogen Energy*

2. Trupti K. Gajaria, Shweta D. Dabhi, and P. K. Jha "ab initio Energetics and Thermoelectric Profiles of Gallium Pnictide Polytypes"
   Scientific reports, **9**(1), 5884 (2019). DOI: 10.1038/s41598-019-41982-9

3. Trupti K. Gajaria, Basant Roondhe, Shweta D. Dabhi, Piotr Śpiewak, Krzysztof J. Kurzydłowski and Prafulla K. Jha, "Hydrogen Evolution Reaction Electrocatalysis Trends of Confined Gallium Phosphide with Substitutional Defects", Accepted, *Int. J. Hydrogen Energy*

4. Narayan N Som, PMWP Sampath, Shweta D Dabhi, Venu Mankad, Satyam Shinde, MLC Attygalle, Prafulla K Jha "Strain and layer modulated electronic and optical properties of low dimensional perovskite methylammonium lead iodide: Implications to solar cells"
   Solar Energy **173,** 1315-1322 (2018). DOI: 10.1016/j.solener.2018.06.052

5. Hardik L. Kagdada, Shweta D. Dabhi and Prafulla K. Jha "Density Functional Study of Adsorption and Desorption dynamics of Hydrogen in Zirconium doped Aluminium clusters"
   Int. J. Hydrogen Energy **43,** (47) 21724-21731 (2018).
   DOI: 10.1016/j.ijhydene.2018.06.041

6. Khushboo Patel, Basant Roondhe, Shweta D Dabhi, Prafulla K Jha "A new flatland buddy as toxic gas scavenger: A first principles study"
   J. hazardous mater. **351,** 337-345 (2018). DOI: 10.1016/j.jhazmat.2018.03.006

7. Pratik D Patel, Satyam Shinde, Sanjay D Gupta, Shweta D Dabhi, Prafulla K Jha "The first principle calculation of structural, electronic, magnetic, elastic, thermal and lattice dynamical properties of fully compensated ferrimagnetic spin-gapless heusler alloy Zr_2MnGa".
   Comput. Condens. Matter **15,** 61-68 (2018). DOI: 10.1016/j.cocom.2018.02.003

8. Shweta D. Dabhi, Basant Roondhe and Prafulla K. Jha "Nucleobases-decorated boron nitride nanoribbons for electrochemical biosensing: a dispersion-corrected DFT study" *Phys. Chem. Chem. Phys.* **20**, 8943-8950, (2018).
   DOI: 10.1039/C7CP08145F

9. Sharad Babu Pillai, Shweta D. Dabhi, Prafulla K. Jha "Hydrogen evolution reaction and electronic structure calculation of two dimensional bismuth and its alloys" DOI: 10.1016/j.ijhydene.2018.04.009
   Int. J. Hydrogen Energy **43,** (47) 21649-21654 (2018).

10. Vaishali Sharma, Narayan Som, Dr. Shweta D Dabhi, Prof. Prafulla K Jha "Tailoring the Electronic and Magnetic Properties of Peculiar Triplet Ground State Polybenzoid "Triangulene"
    Chem. Select **3,** 2390-2397 (2018). DOI: 10.1002/slct.201703054

11. Basant Roondhe, Shweta D. Dabhi, and Prafulla K. Jha "Sensing Properties of Pristine Boron Nitride Nanostructures towards Alkaloids: A First Principles Dispersion corrected Study"
    Appl. Surf. Sci. **441,** 588-598 (2018). DOI: 10.1016/j.apsusc.2018.01.249

12. Narayan N. Som, Venu Mankad, Shweta D. Dabhi, Anjali Patel and Prafulla K. Jha "Magnetic Behavior Study of Samarium Nitride using Density Functional Theory"
    J. Magn. Magn. Mater. **448,** 186-191 (2017). DOI: 10.1016/j.jmmm.2017.10.019

13. Shweta D. Dabhi and Prafulla K. Jha "Tuning of electronic properties and dynamical stability of graphene oxide with different functional groups"
Physica E **93,** 332-338 (2017). DOI: 10.1016/j.physe.2017.07.002

14. S. Pangannaya, Neethu P. P, Shweta Dabhi, Venu Mankad, Prafulla K. Jha, Satyam Shinde and Darshak R. Trivedi; "Spectral and DFT studies of anion bound organic receptors: Time dependent studies and logic gate applications"
Beilstein J. of Organic Chemistry **13,** 222-238 (2017). DOI: 10.3762/bjoc.13.25

15. Showkat H. Mir, Prakash C. Jha, M. S. Islam, Amitava Banarjee, Wei Luo, Shweta D. Dabhi, Prafulla K. Jha and R. Ahuja; "Static and Dynamical Properties of heavy actinide Monopnictides of Lutetium"
Scientific Reports **6,** 29309 (2016). DOI: 10.1038/srep29309

16. Shweta D. Dabhi and Prafulla K. Jha; "Diameter dependent phonon calculations of ultrathin armchair Boron Nitride nanotubes from ab-initio calculations"
Materials Research Express **3,** 085015 (2016). DOI: 10.1088/2053-1591/3/8/085015

17. Shweta D. Dabhi, Deepika Shrivastava, Prafulla K. Jha and Sankar P. Sanyal; "On possibility of superconductivity in SnSb: A first principle study"
Physica C **528,** 56 (2016). DOI: 10.1016/j.physc.2016.07.012

18. Shweta D. Dabhi and Prafulla K. Jha; First principles study for thermodynamic properties of wurtzite Indium Pnictides;
J. Therm. Anal. Calorim. **124,** 1341 (2016). DOI: 10.1007/s10973-016-5298-9

19. S. H. Mir, P. C. Jha, Shweta Dabhi and Prafulla K. Jha, Ab initio study of phase stability, lattice dynamics and thermodynamic properties of Magnesium Chalcogenides;
Mater. Chem. Phys. **175,** 54 (2016). DOI: 10.1016/j.matchemphys.2016.02.066

20. Shweta D. Dabhi and Prafulla K. Jha; Stability, Phonon dispersion and specific heat of solid Poly(vinyl Alcohol) using density functional theory;
Polymer **81,** 45 (2015). DOI: 10.1016/j.polymer.2015.11.009

21. Shweta D. Dabhi and Prafulla K. Jha; Ab initio study of strained wurtzite InAs nanowires: engineering indirect direct band gap transition through size and uniaxial strain;
RSC Advances **5,** 89993 (2015). DOI: 10.1039/c5ra16512a

22. Shweta D. Dabhi and Prafulla K. Jha; Phonon Dispersion and Raman Spectra of Wurtzite InAs under Pressure;
J. Phys. Chem. Solids **83,** 70 (2015). DOI: 10.1016/j.jpcs.2015.03.014

23. Shweta Dabhi, Venu Mankad and Prafulla K. Jha; A First Principles Study of Phase Stability, Bonding, Electronic and Lattice Dynamical Properties of Beryllium Chalcogenides at high pressure;
J. of Alloys and Comp. **617,** 905 (2014). DOI: 10.1016/j.jallcom.2014.08.035

24. Shweta D. Dabhi, Sanjay D. Gupta and Prafulla K. Jha; Structural, Electronic, Mechanical and Dynamical Stability of Graphene Oxides: A First Principles Study;
J. Appl. Phys. **115**, 203517 (2014). DOI: 10.1063/1.4878938

FULL PAPERS IN CONFERENCE PROCEEDINGS

1. Vaishali Sharma, Shweta D. Dabhi, Satyam Shinde and Prafulla K. Jha, Tuning electronic properties of graphene nanoflake polyaromatic hydrocarbon through molecular charge-transfer interactions;
AIP Conf. Proc. **1961**, 030031 (2018). DOI: 10.1063/1.5035233

2. Hardik L. Kagdada, Shweta D. Dabhi, and Prafulla K. Jha, Bandgap tuning and enhancement of seebeck coefficient in one dimensional GeSe;
AIP Conf. Proc. **1942**, 110010 (2018); DOI: 10.1063/1.5028993

3. 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 Conf. Proc. **1832,** 090043 (2017). DOI: 10.1063/1.4980596

4. Sharad B. Pillai, Som Narayan, Shweta D. Dabhi, Prafulla K. Jha, First Principle Calculation of Two Dimensional Antimony And Antimony Arsenide;
AIP Conf. Proc. **1731,** 090024 (2016). DOI: 10.1063/1.4947988

5. Medha D. Pandya, Shweta D. Dabhi, Prafulla K. Jha, Rakesh Rawal; Targeting MLL-CXXC domain with Synthetic CpG dinucleotides: Docking and Molecular dynamics Simulation based approach;
Advanced Materials Research **1141,** 115-120 (2016).
DOI: 10.4028/www.scientific.net/AMR.1141.115

6. Shweta D. Dabhi and Prafulla K. Jha, Tuning the Electronic Band Gap of Graphene by Oxidation; *AIP Conf. Proc.* **1665,** 090013 (2015). DOI: 10.1063/1.4917993

7. Shweta Dabhi and Prafulla K. Jha; Structural and electronic properties of poly(vinyl alcohol) using density functional theory;
AIP Conf. Proc. **1591,** 1133 (2014). DOI: 10.1063/1.4872878

RESEARCH INTEREST

My research work includes the prediction of the physical and chemical properties of different materials using ab-initio computational techniques based on Density Functional Theory. The systems of interests are various Hybrid nanostructures which are functionalized graphene, graphene oxide (GO) and boron nitride (BN) based nanostructures. Variety of GO structures having different functional groups and stoichiometric C:O ratio are studied. Interaction of GO with water molecules, polymer and nanoclusters are also investigated.

Using the state-of-art density functional theory, I have studied structural, electronic and vibrational properties of hexagonal two dimensional BN sheet (h-BN), BN nanotube (BNNT), and BN nano ribbon (BNNR). Currently, I am working on the nature of interactions of h-BN, BNNT and BNNR functionalized with biomolecules and the effect on geometries, adsorption energy and their electronic, structural and charge transfer properties. High pressure phase transition and vibrational dynamics (including phonon, Raman and electron-phonon properties) of bulk systems like Chalcogenides, Pnictides and some Polymers are also studied.

SKILLS AND EXPERTISE

- Programming Languages like C++, Fortran and Python
- Simulation Packages like Quantum Espresso, VASP, Gaussian, Gromacs, ATK-VNL
- Visualization Software like XCrySDen, Vesta, GaussView, VMD etc.
- Modeling and simulation of Bulk, Nano systems (including 2D system, 1D systems like nanotube, nanowire etc.), Polymers and hybrid systems.
- Using the state of art density functional theory (DFT), computing properties like electronic, vibrational, magnetic, optical, thermodynamic and including advanced DFT methods like GW and other hybrid functionals.

CONFERENCE PRESENTATIONS

- "Recent Trends in Condensed Matter Physics" at Bose Institute, Kolkata. **(31 Oct-3 Nov 2017)**
  Title: "Adsorption of Poly(vinyl) Alcohol on Graphene and Graphene Oxide: A Dispersion-Corrected DFT Study"

- Workshop on Physical Virology at International Centre for Theoretical Physics (*ICTP*, Trieste, Italy) **(17-21 July 2017)**
  Title: "Quantum Mechanical Study of Interaction of Nucleobases with Boron Nitride Nanoribbon"

- International Conference on Drug Design at JNU, New Delhi **(7-9 Apr 2017)**
  Title: "A Theoretical Investigation of Amino-acid Functionalized Boron Nitride Nanostructures in 1D and 2D"

- 6th International Conference on Perspectives in Vibrational Spectroscopy at Lucknow **(5-8 Nov 2016)**
  Title: "Structural, Electronic and Vibrational Study of Graphene Oxide and Poly(vinyl alcohol) Nanocomposite" (*Oral presentation*)

- National Conference on Recent Trends in Science of Materials at The M. S. University of Baroda, Vadodara **(28-30 Dec 2015)**
  Title: "Diameter and Strain Dependent Electronic Properties of Indium Arsenide Nanowire" (*Oral Presentation*)

- 4th Nano Today Conference at Dubai, UAE. Organized by Elsevier **(6-10 Dec 2015)**
  Title: "Diameter Dependent Electronic and Vibrational Properties of Armchair Boron Nitride Nanotubes"

- International conference on Diamond and Carbon Materials at Bad Homburg, Germany. Organized by *Elsevier* **(6-10 Sep 2015)**
  Title: "Understanding Interactions of Graphene Oxide with Water Using A Density Functional Theory"

- International Photovoltaic Solar Energy Conference: Solar Asia – 2015 at S. P. Pune University, Pune (*Oral Presentation*) **(30 July-1 Aug 2015)**
  Title: "Electronic and vibrational analysis of oxidized graphene: Ab-initio study"

- 59th DAE-Solid State Physics Symposium at VIT University, Vellore **(16-20 Dec 2014)**
  Title: "Tuning the Electronic Band Gap of Graphene by Oxidation"

- SERB School on "Density Functional Theory and Beyond: Computational Materials Science and Materials Design" at the M. S. University of Baroda, Vadodara (*Oral Presentation*) **(24 Nov-13 Dec 2014)**
  Title: "Electronic and Vibrational Properties of Graphene Oxide"

- MASTANI: Summer School on Materials Simulation Theory And Numerics at IISER, Pune **(30 June-12 July 2014)**
  Title: "Effect of Epoxy and Hydroxyl Functional Group on Graphene: A Computational Study"

- Asia Sweden meeting on understanding functional materials from lattice dynamics (ASMFLD) at IIT Guwahati **(9-11 Jan 2014)**
  Title: "DFT studies of the interaction of graphene oxide with water"

- 58th DAE-Solid State Physics Symposium at Thapar University, Patiala **(17-21 Dec 2013)**
  Title: "Structural And Electronic Properties Of Poly(vinyl Alcohol) Using Density Functional Theory"

- National conference on "New Trends in Physics and Materials Science" at C.S.A. Govt. P. G. College, Sehore **(25-26 Sep 2013)**
  Title: "Structural, electronic and vibrational properties of Graphene Oxides: A first principles study" (*Oral Presentation*)

WORKSHOP/SEMINARS ATTENDED

- Two days National Conference on "Nanotechnology in Agriculture, Energy & Medicine" at Central University of Gujarat, Gandhinagar **(11-12 March 2016)**
- "8th USPEX workshop" at Shiv Nadar University, Noida **(20-24 Jan 2015)**
- Winter School on "Computational Chemistry" at University of Hyderabad **(2-14 Dec 2013)**
- Workshop on "Computational Nanoscience" at Indian Institute of Science, Bangalore **(20–23 August 2013)**
- Workshop on "Parallel Computing for Scientific Applications" at IUAC, New Delhi **(1-2 March 2013)**