Curriculum Vitae

Darshilkumar Pravinbhai Chodvadiya

Senior Research Fellow (DST-INSPIRE) &
JSPS HOPE Fellow - Japan

DEPARTMENT OF PHYSICS, FACULTY OF SCIENCE, THE MAHARAJA SAYAJIRAO UNIVERSITY OF BARODA, VADODARA – 390002, GUJARAT, INDIA.

E-mail: *darshil9000@gmail.com*

Mobile No.: +91-7777993809

Address for Correspondence:

Darshilkumar Pravinbhai Chodvadiya
131: Virat Nagar Society, Near Spinning Mills, Varachha Road, Kapodara, Surat - 395006, Gujarat, India.
Mobile: +91-7777993809

Personal details:

Nationality	**:** Indian
Date of Birth	**:** 22/02/1996
Marital Status	**:** Unmarried
Languages known	**:** English, Hindi and Gujarati

Education qualifications:

- Pursuing **Ph.D. in Physics**, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat, April-2019.
- **M.Sc. in Physics [Gold Medalist]**, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat, 2018. Class: Distinction
- **B.Sc. in Physics [Gold Medalist],** The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat, 2016. Class: Distinction

Academic achievement:

- Received **Best Oral Presentation Award** at National Workshop on Material Design and Processing, Jawaharlal Nehru University (JNU), New Delhi, from 08th to 10th May, 2023.
- Named as **"JSPS HOPE Fellow"** during **14th HOPE Meeting with Nobel Laureates** organized by **Japan Society for the Promotion of Science (JSPS)** in Tokyo, Japan, from 27th February to 3rd March, 2023.
- **Nominated by** the **Department of Science and Technology** (DST), New Delhi, Govt. of India as a participant for **14th HOPE Meeting with Nobel Laureates** organized by **Japan Society for the Promotion of Science (JSPS)** in Tokyo, Japan, from 27th February to 3rd March, 2023.
- Awarded a **PROM Research Scholarship** through **NAWA (National Agency for Academic Exchange) program at Bialystok University of Technology, Poland** (September 2022). Visiting period to Poland: 6th to 13th November, 2022.
- Awarded **INSPIRE FELLOWSHIP as Senior Research Fellow (SRF)** by Department of Science and Technology, Govt. of India (28th April 2021 onwards)

- Received **BEST POSTER AWARD** in 2nd International Conference on Recent Trends in Environment and Sustainable Development (RTESD-2019), Vivekananda Global University, Jaipur, India (October 2019).
- Awarded **INSPIRE FELLOWSHIP as Junior Research Fellow (JRF)** by Department of Science and Technology, Govt. of India (28th April 2019 to 28th April 2021).
- Awarded (1) PROF. D. V. GOGATE GOLD MEDAL and (2) PROF. S. K. SHAH GOLD MEDAL at 67th Convocation of The Maharaja Sayajirao University of Baroda, Vadodara – 390002, Gujarat, India held on 27th January, 2019 (**M.Sc. Physics Gold Medalist**).
- Qualified **Gujarat State Eligibility Test** (**GSET**) for Assistant Professor on 7th December, 2018.
- Awarded **(1) PROFESSOR GOGATE PHYSICS PRIZE and (2) DR. M.S. PATEL PRIZE** for securing the highest number of marks at Third year B.Sc. Physics examination.
- Awarded SHRI SHANKARLAL MANEKLAL CHOKSI GOLD MEDAL at 65th Convocation of The Maharaja Sayajirao University of Baroda, Vadodara – 390002, Gujarat, India held on 17th December, 2016 (**B.Sc. Physics Gold Medalist**).

List of Publication in Journals:

1. **Darshil Chodvadiya**, Shreya Kanabar, Brahmananda Chakraborty, and Prafulla K. Jha. "Exploring the hydrogen storage possibility of the pristine, defected and metals decorated o-B_2N_2 monolayers: Insights from DFT simulations." *(Status: Submitted to Journal)*.

2. Jay Panchal, Apeksha Gauswami, **Darshil Chodvadiya,** Harendrasinh Jadeja and Prafulla K. Jha. "Adsorption Performance of CO, NO and NH_3 Hazardous Gas Molecules over B_9N_9 and Al_9N_9 Nanoclusters: Acumen from Density Functional Theory." *(Status: Submitted to Journal).*

3. Bhautik R. Dhori, **Darshil Chodvadiya,** and Prafulla K. Jha. "Evidence of topological phase transition with excellent catalytic activity in AgCaAs Heusler alloy: A first-principles investigation." ***Journal of Physical Chemistry C*** **(2023)**: 127(31), 15461–15473.

4. Paras Patel, Saurav Patel, **Darshil Chodvadiya**, Madhavi H. Dalsaniya, Dominik Kurzydłowski, Krzysztof J. Kurzydłowski, and Prafulla K. Jha. "A density functional theory study on the assessment of α-CN and α-CP monolayers as anode material in Li-ion batteries." ***Journal of Energy Storage (2023)***: 71, 108074.

5. Shardul Vadalkar, **Darshil Chodvadiya**, Narayan N. Som, Keyur N. Vyas and Prafulla K. Jha. "Cyclo[18]carbon as a Hazardous Gas Scavenger: Effect of Boron and Nitrogen Doping on Molecular Adsorption." ***ChemistrySelect (2023)***: 8(23), e202204862.

6. Pratikkumar Lakhani, **Darshil Chodvadiya**, Prafulla K. Jha, Vivek Kumar Gupta, Damian Trzybiński, Krzysztof Wozniak, Krzysztof Kurzydłowski, U. K. Goutam, Himanshu Srivastava, Chetan K. Modi. "DFT stimulation and experimental insights of chiral Cu(II)-salen scaffold within the pocket of MWW-zeolite and its catalytic study." ***Physical Chemistry Chemical Physics (2023)*****:** 25, 14374-14386.

7. **Darshil Chodvadiya**, Brahmananda Chakraborty, and Prafulla K. Jha. "Transition metal atoms anchored 2D holey graphyne for hydrogen evolution reaction: Acumen from DFT simulation." ***International Journal of Hydrogen Energy (2023)*****:** 48(48), 18326-18337.

8. **Darshil Chodvadiya**, Madhavi H. Dalsaniya, Narayan N. Som, Brahmananda Chakraborty, Dominik Kurzydłowski, Krzysztof J. Kurzydłowski, and Prafulla K. Jha. "Defects and doping engineered two-dimensional o-B_2N_2 for hydrogen evolution reaction catalyst: Insights from DFT simulation." ***International Journal of Hydrogen Energy (2023)*****:** 48(13), 5138-5151.

9. Paras Patel, Saurav Patel, **Darshil Chodvadiya**, Madhavi H. Dalsaniya, Dominik Kurzydłowski, and Prafulla K. Jha. "Two-Dimensional α-SiX (X = N, P) Monolayers as Efficient Anode Material for Li-Ion Batteries: A First-Principles Study**.**" ***ACS Applied Nano Materials (2023)*****:** 6(3), 2103-2115**.**

10. **Darshil Chodvadiya**, Prafulla K. Jha, and Brahmananda Chakraborty. "Theoretical inspection of Ni/α-SiX (X= N, P, As, Sb, Bi) Single-Atom catalyst: Ultra-high performance for hydrogen evolution reaction." ***International Journal of Hydrogen Energy (2022)*****:** 47(99), 41733-41747.

11. Sourav Kanti Jana, **Darshil Chodvadiya**, Narayan N. Som, and Prafulla K. Jha. "A quantum mechanical prediction of C_{24} fullerene as a DNA nucleobase biosensor." ***Diamond and Related Materials (2022)*****:** 129, 109305.

12. **Darshil Chodvadiya**, Ujjawal Jha, Piotr Śpiewak, Krzysztof J. Kurzydłowski, and Prafulla K. Jha. "Potential anodic application of 2D h-AlC for Li and Na-ions batteries." ***Applied Surface Science (2022)*****:** 593, 153424.

13. Nayana Shekh, **Darshil Chodvadiya**, and Prafulla K. Jha. "Rational design of h-AlC monolayer as anode material for Mg-ion battery: A DFT study." ***Energy Storage (2022)*****:** 5(3), e415.

14. Saurav Patel, Paras Patel, **Darshil Chodvadiya**, Narayan N. Som, and Prafulla K. Jha. "Adsorption performance of C_{12}, B_6N_6 and Al_6N_6 nanoclusters towards hazardous gas molecules: A DFT investigation for gas sensing and removal application." ***Journal of Molecular Liquids (2022)***: 352, 118702.

15. Shardul Vadalkar, **Darshil Chodvadiya**, Narayan N. Som, Keyur N. Vyas, Prafulla K. Jha, and Brahmananda Chakraborty. "An Ab-initio Study of the C_{18} nanocluster for Hazardous Gas Sensor Application." ***ChemistrySelect (2022)***: 7(3), e202103874.

16. **Darshil Chodvadiya**, Narayan N. Som, Prafulla K. Jha, and Brahmananda Chakraborty. "Enhancement in the catalytic activity of two-dimensional α-CN by B, Si and P doping for hydrogen evolution and oxygen evolution reactions." ***International Journal of Hydrogen Energy (2021)*****:** 46(43), 22478-22498.

17. Trupti K. Gajaria, **Darshil Chodvadiya**, and Prafulla K. Jha. "Density functional theory investigation of thermal conductivity in α-CN and α-CP monolayers: Implications for

thermal management of electronic devices." ***ACS Applied Nano Materials (2021)*****:** 4(5), 4474-4483.

List of Publication in Conference Proceedings:

1. Shardul Vadalkar, **Darshil Chodvadiya**, Keyur N. Vyas, and Prafulla K. Jha. "Adsorption of HCN on pristine and Al/Si/P decorated C_{18} nanocluster: a first principles study." ***Materials Today: Proceedings (2022)***: 67, 229-237.
2. **Darshil Chodvadiya**, Prafulla K. Jha and Brahmananda Chakraborty. "Introduction of Defects in 2D α-SiN for Improvement in Hydrogen Evolution Reaction Activity: A DFT Study." ***Proceedings of the 65th DAE Solid State Physics Symposium (2021)*****:** 574-575.
3. **Darshil Chodvadiya**, Sharad Babu Pillai, Brahmananda Chakraborty, and Prafulla K. Jha. "Strain effect on Mexican-hat dispersion and electronic band gap of 2D α-CN." ***AIP Conference Proceedings (2020)*****:** 2265(1), 030377.

Research Interests:

- Materials design and modelling of 3D, 2D, 1D and 0D materials for various applications using Density Functional Theory.
- Investigation of various nanomaterials for energy applications (for example: hydrogen production, hydrogen storage, batteries and thermoelectric) using Density Functional Theory.
- Exploring the sensing applications (for example: toxic gas molecule, bio-molecules and etc.) of nanomaterials using Density Functional Theory.

Skills and Expertise:

- Programming Languages: Fortran and Python.
- Simulation Packages: Quantum Espresso, Gaussian and VASP.
- Visualization Software: XCrySDen, VESTA, GaussView and GaussSum.
- Modelling and simulation of Bulk to Nano materials.
- Using density functional theory (DFT), computing properties like electronic, vibrational, magnetic, optical and thermodynamic.

Conference/Workshop/Seminar presentations:

1. **Darshil Chodvadiya,** "Assessing the Suitability of α-CM (M = N, P) Monolayers as Anode Material in Li-ion Batteries: A DFT Study", **National Workshop on Material Design and Processing at Jawaharlal Nehru University (JNU), New Delhi**, **India,** from 08th to 10th May, 2023 (Oral Presentation).
2. **Darshil Chodvadiya,** "Defects and Doping Engineered Two-dimensional o-B_2N_2 for Hydrogen Evolution Reaction Catalyst: Insight from DFT simulations", **14th HOPE Meeting with Nobel Laureates** organized by **Japan Society for the Promotion of Science (JSPS)** in Tokyo, Japan, from 27th February to 3rd March, 2023 (Oral and Poster Presentation).
3. **Darshil Chodvadiya**, "An ab-initio study on B_9N_9 nanocluster for application as atmospheric gas (CO, NO, NH_3) sensor", **66th DAE Solid State Physics Symposium at**

Birla Institute of Technology Mesra, Ranchi, Jharkhand, India, December 2022 (Poster Presentation).

4. **Darshil Chodvadiya**, "Introduction of Defects in 2D α-SiN for Improvement in Hydrogen Evolution Reaction Activity: A DFT Study", **65th DAE Solid State Physics Symposium at Bhabha Atomic Research Centre, India,** December 2021 (Poster Presentation).
5. **Darshil Chodvadiya,** "Theoretical Inspection of Ni/α-SiX (X=N, P, As, Sb, Bi) Single-Atom Catalyst: Ultra-High Performance for Hydrogen Evolution Reaction", **International Conference on Condensed Matter and Device Physics, Department of Physics, School of Technology, PDEU, Gandhinagar, India,** September 2021 (Oral Presentation).
6. **Darshil Chodvadiya,** "Exploring Thermoelectric Transport through Carbon Pnictide Monolayers", **International conference on electron-phonon coupling and thermoelectric efficiency, online at University of the Basque country, Spain,** November 2020 (Oral Presentation).
7. **Darshil Chodvadiya,** "Strain effect on Mexican-hat dispersion and electronic band gap of 2D α-CN", **64th DAE Solid State Physics Symposium at Indian Institute of Technology Jodhpur, Rajasthan, India,** December 2019 (Poster Presentation).
8. **Darshil Chodvadiya,** "Revealing the Size Effect on Reactivity of Carbon Monoxide over Yttrium Doped Sc_n (where n =2 to 8) Nanoclusters", **2nd International Conference on Recent Trends in Environment and Sustainable Development, Vivekananda Global University Jaipur, India,** October 2019 (Poster Presentation).

Workshop/Seminars Attended:

1. Attended a workshop on "**Training Program for Developing Skills on Material Characterization Techniques**" under STUTI at Department of Physics, The M. S. University of Baroda, Vadodara, Gujarat, India, 21st to 27th November, 2023.
2. Attended a seminar on "**Machine Learning in Chemistry: Now and in the Future**" organized by American Chemical Society (ACS), May 2021.
3. Attended a workshop on "**Advanced Analytical Techniques for Elemental Analysis**" at Department of Chemistry, The M. S. University of Baroda, Vadodara, Gujarat, India, December 2019.

References:

Prof. Prafulla K. Jha (Research Guide)
Head, Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara-390002, Gujarat, India.
Phone: +91-265-2795339 (O) and +91-9825032877 (M)
Email: prafullaj@yahoo.com

Dr. Brahmananda Chakraborty (Research Co-Guide)
Scientist G, High Pressure and Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, India.
Phone: +91-2225592057 (O) and +91-987111453 (M)
Email: brahma@barc.gov.in