

CURRICULUM VITAE 2018 Feb

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DEOBRAT SINGH

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RESEARCH EXPERIENCE/

RESEARCH INTEREST

2014-Present

S.V. National Institute of Technology
Surat

2-Dimensional Materials and Its Applications

1. The research work deals with the basics of condense matter physics using Density Functional Theory based on first principal calculations.
2. The research work mainly focuses on structural, vibrational, electronic, opto-electronic and magnetic properties of 2D monolayer/multilayer materials.
3. Investigations are done for structural and electric field-induced changes in electronic properties of mono and multilayer material using Density Functional Theory (DFT) with the help of Quantum Espresso (QE) and Vienna Ab initio Simulation Package (VASP).
4. This research work has achieved various applications and alternative to various materials in real life. For example, HfS₂ is found to be suitable as photocatalysts for water splitting, Si₂BN as an efficient material for hydrogen storage, etc.

January 2018-Present

Organization

Area

Main activities and responsibilities

Assistant Professor

Government college of engineering and technology
Bikaner, Rajasthan, India

- Conducting lectures in bachelor's level in engineering.
- Organizing and managing student research progress.
- Developing research facilities in the department.
- Conducting laboratory sessions.

June 2017- January 2018

Organization

Area

Main activities and responsibilities

Assistant Professor

Marwadi Education Foundation Group of Foundations (MEFGI)
Rajkot, Gujarat, India

- Conducting lectures in bachelor's and master's level in engineering and science.
- Organizing and managing student learning progress.
- Exploring new and innovative real-world problem and solving the by

July 2010-2011
Organization
Area
Main activities and responsibilities

computational tools.

- Conducting laboratory sessions and explaining applications to students.

Teaching Assistant

City Montessori Group of School,
Balrampur, Uttar Pradesh, India

- Conducting physics lectures for students of class 12th.
- Demonstrated ability to assist lead teachers by performing secretarial and one-on-one lessons importation tasks.
- Proven success in using educational materials and resources.
- Track record of creating and maintaining effective student-teacher relationships.
- Coordinates students in recreational activities at school.

NATIONAL ACHIEVEMENTS AND

AWARDS

June-2014

Lecturer-ship in National Eligibility Test (NET)

Council of Scientific and Industrial Research, University Grand
Commission (CSIR-UGC), Delhi, India

2014

Graduate Aptitude Test for Engineering (GATE)

Indian Institute of Technology (IIT), Kharagpur, India

December-2013

Junior Research Fellow (JRF-NET)

Council of Scientific and Industrial Research, University Grand
Commission (CSIR-UGC), Delhi, India

EDUCATION AND TRAINING

2014-Present

Institute
Area

Ph.D. (Synopsis Submitted)

S.V. National Institute of Technology
Surat, Gujarat, India

2008- 2010

Institute
Area

M.Sc. in Physics

M. L. K. P. G. College
Balrampur, Uttar Pradesh, India

2005-2008

Institute
Area

B.Sc. in Physics

M. L. K. P. G. College
Balrampur, Uttar Pradesh, India

2004-2005

Institute

Area

Intermediate (Class 12th)

H. R. Inter College

Khalilabad, Uttar Pradesh, India

2002-2003

Institute

Area

High School (Class 10th)

A. K. Inter College

Khalilabad, Uttar Pradesh, India

LANGUAGES KNOWN

Hindi, English

COMPUTER SKILLS

Operating systems
Software Skills and
Computational Tools

Linux and Microsoft Windows

Microsoft Office, Origin, LaTeX, FORTRAN, Mathematica, MATLAB,
VASP, Quantum Espresso, VESTA, etc.

PUBLICATIONS

INTERNATIONAL JOURNALS (SCI Journals)

1. Prabal Dev Bhuyan, Sanjeev K. Gupta, **Deobrat Singh**, Yogesh Sonvane, P. N. Gajjar. "Electronic, Magnetic and Optical Properties of 2D Metal Nanolayers: A DFT Study." *Metals and Mater. Internat.*, 2018, (Accepted) **(Impact Factor: 1.889)**
2. **Deobrat Singh**, S. Kansara, S. K. Gupta, and Y. Sonvane. "Single-layer of Carbon-Phosphide as a High Performance for Optoelectronic Devices." *J. Mater. Sci.*, 2018 (DOI: 10.1007/s10853-018-2126-6). **(Impact Factor: 2.599)**
3. Kavita Pandey, **Deobrat Singh**, Sanjeev Kumar Gupta, Pankaj Yadav, Yogesh Sonvane, Igor Lukačević, Manjeet Kumar, Manoj Kumar, Rajeev Ahuja, "Improving electron transport in the hybrid perovskite solar cells using CaMnO₃-based buffer layer" *Nano Energy*, 2018 (DOI: 10.1016/j.nanoen.2018.01.009) **(Impact Factor: 12.34)**
4. **Deobrat Singh**, Sanjeev K Gupta, Yogesh Sonvane, Satyaprakash Sahoo, "Modulating the electronic and optical properties of monolayer arsenene phases by organic molecular doping" *Nanotechnology*, 2017 (DOI: 10.1088/1361-6528/aa9430) **(Impact Factor: 3.44)**
5. **Deobrat Singh**, Sanjeev K. Gupta, Yogesh Sonvane, and Rajeev Ahuja. "High performance material for hydrogen storage: Graphenelike Si₂BN solid." *Int. J. Hydrogen Energy*, 2017, 42, 22942-22952. **(Impact Factor: 3.582)**
6. Shivam Kansara, **Deobrat Singh**, Sanjeev K. Gupta and Yogesh Sonvane, "Ab Initio Investigation of Vibrational, Optical Properties and Thermodynamics of Yttrium Arsenide." *J. Electron. Mater.*, 2017, 46,

- 5670–5676. **(Impact Factor: 2.599)**
7. Prabal Dev Bhuyan, **Deobrat Singh**, Shivam Kansara, Pritam Yadav, Sanjeev K. Gupta, Yogesh Sonvane, Sanjeeb K. Rout, and Ela Sinha, Experimental and theoretical analysis of electronic and optical properties of MgWO₄, J. Mater. Sci., 2017, 52, 4934–4943. **(Impact Factor: 2.599)**
 8. **Deobrat Singh**, Yogesh Sonvane, Shivam Kansara, and P. B. Thakor. "Thermal Conductivity and Thermoelectric Power of Some Transition Metals in Liquid Phase." Adv. Sci. Lett., 2016, 22(11), 3944-3947. **(Impact Factor: 1.253)**
 9. Yogesh Sonvane, **Deobrat Singh**, Sanjeev K. Gupta and Shivam Kansara, "Temperature & Size Dependent Thermal Conductivity of Graphene Nanoribbons Description for Phonon Dispersion and Polarization" Adv. Sci. Lett., 2016, 22(11), 3916-3918. **(Impact Factor: 1.253)**
 10. H. R. Mahida, **Deobrat Singh**, Yogesh Sonvane, Sanjeev K. Gupta, and P. B. Thakor, "MgF₂ Monolayer as an Anti-Reflecting Material" Solid State Commun., 2016, 252, 22-28. **(Impact Factor: 1.554)**
 11. Shivam Kansara, **Deobrat Singh**, Sanjeev K. Gupta, and Yogesh Sonvane. "Density functional Studies of structural, electronic and vibrational properties of palladium oxide." Solid State Commun., 2016, 245, 36-41. **(Impact Factor: 1.554)**
 12. Kavita Pandey, Pankaj Yadav, **Deobrat Singh**, Sanjeev K. Gupta, Yogesh Sonvane, Igor Lukačević, Joondong Kim and Manoj Kumar, "First step to investigate nature of electronic states and transport in flower-like MoS₂: Combining experimental studies with computational calculations" Sci. Rep., 2016, 6, 32690. **(Impact Factor: 5.228)**
 13. Sanjeev K. Gupta, **Deobrat Singh**, Kaptan Rajput and Yogesh Sonvane, "Germanene: New Electronic Gas Sensing Material" RSC Adv., 2016, 6, 102264-102271. **(Impact Factor: 3.108)**
 14. **Deobrat Singh**, Sanjeev K. Gupta, Yogesh Sonvane, Ashok Kumar and Rajeev Ahuja, "2D-HfS₂ as an efficient Photocatalyst for Water Splitting" Catal. Sci. Technol., 2016, 6, 6605-6614. **(Impact Factor: 5.772)**
 15. **Deobrat Singh**, Sanjeev K. Gupta, Yogesh Sonvane and I. Lukačević, "Antimonene: a monolayer material for ultraviolet optical nanodevices" J. Mater. Chem. C, 2016, 4, 6386-6390. **(Impact Factor: 5.256)**
 16. **Deobrat Singh**, Sanjeev K. Gupta, Igor Lukačević, and Yogesh Sonvane, "Indiene 2D Monolayer: a New Nanoelectronic Material" RSC Adv., 2016, 6, 8006-8014. **(Impact Factor: 3.108)**

**INTERNATIONAL/NATIONAL
CONFERENCE PROCEEDINGS
(Conference papers)**

1. **Deobrat Singh**, Nisha Singh, Sanjeev K Gupta, Yogesh Sonvane, "Effect on electronic and optical properties of Frenkel and Schottky defects in HfS_2 monolayer" AIP Conference Proceedings, 2017 (Accepted)
2. Mohini Ramwala, **Deobrat Singh**, Sanjeev K. Gupta, Yogesh Sonvane, "Metal-Mott Insulator Transition of SrMnO_3 by Fluorine Doping" AIP Conference Proceedings, 2017, 1832, 090031.
3. Sagar Parekh, **Deobrat Singh**, Sanjeev K. Gupta, Yogesh Sonvane, "Structural, electronic and Ferroelectric properties of BaReO_3 " AIP Conference Proceedings, 2017, 1832, 090033.
4. **Deobrat Singh**, Sanjeev K. Gupta, Yogesh Sonvane, "Effect of oxygen atom on electronic and optical properties of 2D monolayer of PtS_2 " AIP Conference Proceedings, 2017, 1832, 090024.
5. Sagar Parekh, Mohini Ramwala, Ruchi Rathod, **Deobrat Singh**, Sanjeev K. Gupta, Yogesh Sonvane," Structural, Electronic and Ferroelectric Properties of BaTcO_3 " AIP Conference Proceedings, 2017, 1837, 040030.
6. H. R. Mahida, **Deobrat Singh**, Sanjeev K. Gupta, Yogesh Sonvane, and P. B. Thakor. "Electronic and transport properties of fluorite structure of $\text{La}_2\text{Ce}_2\text{O}_7$." AIP Conference Proceedings, 2017, 1832, 090038.
7. **Deobrat Singh**, Yogesh Sonvane, and P. B. Thakor. "Vibrational Properties of Zr–Ni Metallic Glasses." Materials Today: Proceedings, 2016, 3(9), 3137-3143.
8. **Deobrat Singh**, Yogesh Sonvane, and P. B. Thakor, Mechanical properties of 4d transition metals in molten state. AIP Conference Proceedings, 2016, 20408, 1728.
9. Pinank Jariwala, **Deobrat Singh**, Yogesh Sonvane, Sanjeev K. Gupta and P.B. Thakur, "First-Principle Study of Structural and Electronic properties of Pyramidal Silicon Nanowire" AIP Conference Proceedings, 2016, 1731, 090042.
10. **Deobrat Singh** and Yogesh Sonvane, "Theoretical investigation of structural and electronic properties of Ultrathin Nickel Nanowire" AIP Conference Proceedings, 2016, 1724, 020134.
11. **Deobrat Singh**, Sanjeev K. Gupta and Yogesh Sonvane, "Structural and Opto-Electronic Properties of 2D AlSb Monolayer" AIP Conference Proceedings, 2016, 1731, 120018.

**NATIONAL/ INTERNATIONAL
WORKSHOP/CONFERENCE
ATTENDED AND PRESENTED**

1. A Research Paper (Poster Presentation) entitled "**Effect on electronic and optical properties of Frenkel and Schottky defects in HfS_2 monolayer**" in the **62nd DAE Solid State Physics Symposium**, Bhabha Atomic Research Centre, Anushaktinagar, Mumbai. (26-30th December-2017).

2. A Research Paper (Poster Presentation) entitled “**Effect of oxygen atom on electronic and optical properties of 2D monolayer of PtS₂**” in the **61st DAE Solid State Physics Symposium**, KIIT University, Bhubaneswar. (26-30th December-2016).
3. **Nanotechnology: Insights into Properties of Materials from Computational Modeling Methods, GIAN-2016**, Guru Jambheshwar University of Science and Technology, Hisar, Haryana. (16-20th October-2016).
4. A Research Paper (Poster Presentation) entitled “**Structural and Opto-Electronic Properties of 2D AlSb Monolayer**” in the **60th DAE Solid State Physics Symposium**, Amity University UP, Noida. (21-25th December-2015).
5. **DAE-BRNS 3rd National Workshop on Materials Chemistry-NWMC-2015**, BARC Mumbai. (20-21st November-2015)
6. A Research Paper (Poster Presentation) entitled “**Temperature & Size Dependent Thermal Conductivity of Graphene Nanoribbons Description for Phonon Dispersion and Polarization**” in the **8th National Conference on Thermophysical Properties**, Department of Physics, MNIT, Jaipur. (14-16th December-2015).
7. A Research Paper (Poster Presentation) entitled “**Mechanical properties of 4d transition metals in molten state**” in the **International Conference on Condensed Matter & Applied Physics**, Department of Physics, Govt. Engineering College Bikaner. (30-31st October-2015).
8. **SERB School on Density Functional Theory and Beyond: Computational Materials Science and Materials Design**, Department of Physics, Faculty of Science, The M.S. University of Baroda, Vadodara-390002, Gujarat. (24th November-13th December-2014).