

Curriculum Vitae

Durgesh Kumar Sharma

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Professional Summary

A highly motivated researcher driven to elucidate the novel properties of 2D and bulk materials. Proficient in performing a variety of calculations based on density functional theory, including electronic structure, optical properties, and non-trivial Berry phase. Quick learner and can work in collaboration with experimental groups.

Research Experience

April 2014-May 2015	Research Scholar	MJP Rohilkhand University
June 2015-May 2018	Project Assistant	MJP Rohilkhand University
June 2018-July 2019	Sr. Research Scholar	MJP Rohilkhand University
April 2021-April 2023	National Post Doctoral Fellow	JNCASR, India
April 2023-June 2023	Research Associate	JNCASR, India
Sept. 2023-June 2025	Post Doctoral Fellow	MJP Rohilkhand University

Teaching Experience

Aug. 2019-May 2020	Guest Lecturer	MJP Rohilkhand University
Dec. 2020-March 2021	Guest Lecturer	MJP Rohilkhand University
August 2025-Present	Assistant Professor	Gangasheel Mahavidyalaya

Highest Conferred Qualification

Ph.D. in Physics from MJP Rohilkhand University

Ph.D. Thesis Title: "Stability, Electronic, and Optical Properties of 2D Materials: An *ab-initio* Study"

Date of Award: Feb. 04, 2021

Thesis Advisor: Prof. Sudhir Kumar

Expertise/Technical Skills

I can

- predict the dynamical stability, electronic structure, and optical properties of bulk, 2D, and 1D nano ribbons.
- investigate the non-trivial electronic Berry phase and anomalous Hall conductivity in 2D materials.
- predict the transition state and low-energy pathways for the kinetics of ion.
- align the electronic bands with respect to the vacuum level.
- induce defect and can predict the impact of defects (charged/vacancy/antisite/impurity) on the electronic structure and the stability of the material.
- calculate the thermoelectric properties of bulk as well as 2D materials.
- prepare alloys of materials with a minimum energy configuration by doping impurity atoms.
- visualize wave functions/electron charge density.
- predict the transfer of charge between atoms and the electron localization function.

Software Expertise

- Vienna *ab-initio* Simulation Package (VASP)
- Quantum Espresso
- PHONOPY
- Site Occupancy Disorder (SOD) Program
- Wannier90
- Wannier Berry
- VASPBERRY
- Z2Pack
- WannierTools
- VESTA
- Inkscape

Awards

- Awarded by Sri Ram Seva Trust for securing the highest marks at the college level in M.Sc.
- Appreciation certificate for a poster presentation at the conference IWCCMP-2016 at AVB-IIITM Gwalior in February 2016.
- National Post-Doctoral Fellowship by the Science and Engineering Research Board, India, in December 2020.

References

1. Prof. Sudhir Kumar
Applied Physics Department,
M. J. P. Rohilkhand University, Bareilly
email: skumar@mjpru.ac.in
2. Dr. Bhasker Gahtori
Principal Scientist
CSIR-National Physical Laboratory, Dr K. S. Krishnan Marg, New Delhi
email: bhasker@nplindia.org

List of Publications in Journals

1. Band gap engineering of ZnO substituted with nitrogen and fluorine, $\text{ZnO}_{1-3x}\text{N}_{2x}\text{F}_x$: A hybrid density functional study
S. Kumar, **Durgesh Kumar Sharma**, and S. Auluck
RSC Advances **6**, 99088 (2016).
2. Theoretical insight into kesterite and stannite phases of $\text{Cu}_2(\text{Sn}_{1-x}\text{Ge}_x)\text{ZnSe}_4$ based alloys: A prospective photovoltaic materials
S. Kumar, **Durgesh Kumar Sharma**, Bipin Joshi, and S. Auluck
AIP Advances **6**, 125303 (2016).
3. Stability, electronic and optical properties of wurtzite $\text{Cu}_2\text{Cd}_x\text{Zn}_{1-x}\text{SnS}_4$ alloys as photovoltaic materials: First-principles insight
S. Kumar, **Durgesh Kumar Sharma**, and S. Auluck
Physical Review B **94**, 235206 (2016).
4. Magnetism by embedding 3d transition metal atoms into germanene
Durgesh Kumar Sharma, Sudhir Kumar, and Sushil Auluck
Journal of Physics D: Applied Physics **51**, 225006 (2018).
5. Mono and bi-layer germanene as prospective anode material for Li-ion batteries: A first-principles study
Durgesh Kumar Sharma, Sudhir Kumar, Amel Laref, and Sushil Auluck
Computational Condensed Matter **16**, e00314 (2018).
6. Electronic structure, defect properties, and hydrogen storage capacity of 2H-WS₂: A first-principles study
Durgesh Kumar Sharma, Sudhir Kumar, and Sushil Auluck
International Journal of Hydrogen Energy **43**, 23126 (2018).
7. Theoretical characterization of C doped SiGe monolayer
Durgesh Kumar Sharma, Sudhir Kumar, and Sushil Auluck
Journal of Applied Physics **125**, 145703 (2019).
8. Enhancing gas adsorption properties of borophene by embedding transition metals
S. Kumar, Manoj Singh, **Durgesh Kumar Sharma**, and Sushil Auluck
Computational Condensed Matter **22**, e00436 (2020).
9. Influence of defect pairs in Ga-based ordered defect compounds: A hybrid density functional study
Sudhir Kumar, Suman Joshi, **Durgesh Kumar Sharma**, and Sushil Auluck
Canadian Journal of Physics **98**, 770 (2020).
10. Strain induced optoelectronic properties of two dimensional MnPSe₃/WS₂ heterostructure
Durgesh Kumar Sharma, Sudhir Kumar, and Sushil Auluck
Journal of Physics: Condensed Matter **32**, 315501 (2020).
11. Observation of antiferromagnetic ordering from muon spin resonance study and the Kondo effect in a Dy-doped Bi₂Se₃ topological insulator
Vinod Kumar Gangwar, S. Kumar, M. Singh, L. Ghosh, D. Pal, P. Shahi, Y. Uwatoko, E.

Schwier, F. Shimada, **Durgesh Kumar Sharma**, S. Kumar, and S. Chatterjee
Journal of Physics D: Applied Physics **54**, 544302 (2021).

12. Ultrasensitive Boron-Nitrogen-Codoped CVD Graphene-Derived NO₂ Gas Sensor
S. Srivastava, P. Pal, **Durgesh Kumar Sharma**, S. Kumar, T. D. Senguttuvan, Bipin Kumar Gupta
ACS Materials Au **2**, 356 (2022).
13. Role of sintering temperature on electronic and mechanical properties of thermoelectric material: A theoretical and experimental study of TiCoSb half-heusler alloy
A. K. Verma, K. K. Johari, Kriti Tyagi, **Durgesh Kumar Sharma**, P. Kumar, S. Kumar, S. Bathula, S. R. Dhakate, B. Gahtori
Materials Chemistry and Physics **281**, 125854 (2022).
14. In Situ Evolution of Secondary Metallic Phases in Off-Stoichiometric ZrNiSn for Enhanced Thermoelectric Performance
K. K. Johari, **Durgesh Kumar Sharma**, A. K. Verma, R. Bhardwaj, N. S. Chauhan, S. Kumar, M. N. Singh, S. Bathula, B. Gahtori
ACS Applied Materials & Interfaces **14**, 19579 (2022).
15. Lattice Dynamics of Bi_{1.9}Dy_{0.1}Te₃ Topological Insulator
L. Ghosh, V. K. Gangwar, M. Singh, S. V. Kumar, S. Dixit, A. Verma, **Durgesh Kumar Sharma**, S. Kumar, S. Saha, A. K. Ghosh, S. Chatterjee
Physica B: Condensed Matter **640**, 414050 (2022).
16. Realization of Band Convergence in p-Type TiCoSb Half-Heusler Alloys Significantly Enhances the Thermoelectric Performance
A. K. Verma, K. K. Johari, P. Dubey, **Durgesh Kumar Sharma**, S. Kumar, S. Dhakate, C. C. Rangnate, B. Lenoir, and B. Gahtori
ACS Applied Materials & Interfaces **15**, 942 (2023).
17. The charge carrier density modulation in off-stoichiometric ZrNiSn leads to enhanced thermoelectric performance
Kishor Kumar Johari, Ajay Kumar Verma, Naval Kishor Upadhyaya, Radhey Shyam, **Durgesh Kumar Sharma**, Sudhir Kumar, Bhasker Gahtori
Ceramics International **49**, 26558 (2023).
18. In-situ formation of CrB minor phase during reactive spark plasma sintering leads to the enhancement in the electrical transport performance of boron doped chromium disilicide
Manju Yadav, **Durgesh Kumar Sharma**, Kishor Kumar Johari, Naval Kishor Upadhyay, Radhey Shyam, Sudhir Kumar, Saravanan Muthiah, Bhasker Gahtori
Materials Chemistry and Physics **316**, 129004 (2024).
19. Theoretical investigation of gas sensing properties of a monolayer gallene: First-principles insight
Pawan Kumar, Siya Singh, **Durgesh Kumar Sharma**, Sudhir Kumar
Materials Today Communications **40**, 109268 (2024).
20. First-Principles Insights in Designing Two-Dimensional BY_{1-x}Z_x (Y, Z = P, As, and Sb, but Y ≠ Z) Alloys: A Potential Candidate for Thin-Film Optoelectronic Devices

Durgesh Kumar Sharma, Pawan Kumar, Rajeev Ahuja, and Sudhir Kumar
Journal of Physical Chemistry C **130**, 2466 (2026).

List of Publications in Conference Proceedings

1. Band Gap Tuning of $\text{ZnO}_{1-3x}\text{N}_{2x}\text{F}_x$ Alloys: A First Principles Study
S. Kumar, **Durgesh Kumar Sharma**, and S. Auluck
Materials Today: Proceedings **4**, 5700 (2017).
2. Magnetism in mono-layer of germanium
Durgesh Kumar Sharma, Sudhir Kumar, and Sushil Auluck
4th International Conference on Academic Research in Engineering, Management and Information Technology (ICAREMIT-2019), Page 242-246, 16-18 April 2019
ISBN 978-81-933433-5-7

Participation/Paper Presentation in Conferences/Schools/Workshops

1. Participate in “*International Workshop on Futuristic Materials: Characterization Properties and Application in Technology*”, Organized by Applied Physics Department, M. J. P. Rohilkhand University, Bareilly (17-22 July 2014).
2. Participate in “*Winter School on Materials and Processes for Application in Energy and Environment*”, Organized by Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru (15-17 January 2015).
3. Participate in “*International Conference on Multifunctional Materials for Device Applications (ICMDA-2016)*”, Organized by- Department of Physics, National Institute of Technology, Patna (26-28 October 2016).
4. Poster presentation in “*4th International E-Workshop/Conference On Computational Condensed Matter Physics and Material Science (IWCCMP-2016)*”, Organized by- AVB-Indian Institute of Information Technology and Management, Gwalior (18-20 November 2016).
5. Poster presentation in “*International Conference on Emerging Materials and Applications (ICEMA-2017)*”, Organized by- Physics Department, University of Allahabad, Allahabad (20-22 February 2017).
6. Poster Presentation in “*National Conference on Recent Trends in Condensed Matter Physics and Materials Science*”, Organized by- Department of Physics, Banaras Hindu University, Varanasi (15-16 September 2018).
7. Poster presentation in “*International Conference on Advanced Materials (ICAM-2019)*”, Organized by- Centre of Nanoscience and Nanotechnology, Jamia Millia Islamia (A Central University), New Delhi (6-7 March 2019).
8. Oral presentation in “*4th International Conference on Academic Research in Engineering, Management and Information Technology (ICAREMIT-2019)*”, Organized by- Department of Mechanical Engineering F. E. T., M. J. P. Rohilkhand University, Bareilly (16-18 April 2019).

9. Poster presentation in “*International Winter School 2019 on Frontiers in Materials Science*”, Organized by- Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore (2-6 December 2019).
10. Participate in “*Workshop on In silicon Quantum Modelling Studies*”, Organized by Inter-University Accelerator Centre, New Delhi (30 October - 03 November 2022).
11. Poster Presentation in “*International Winter School 2022 on Frontiers in Materials Science*”, Organized by- Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru (05-09 December 2022).
12. Poster Presentation in “*International Conference on Advances in Renewable Energy (CARE-2023)*”, Jointly Organized by HRI, Prayagraj and TIFR-Hyderabad (02-04 February 2023).
13. Poster Presentation in “*New Approaches and Machine learning and Materials Methods for Ab initio calculations (NAMMA-Psi K Workshop)*” Jointly Organized by Jawaharlal Nehru Centre for Advanced Scientific Research and Indian Institute of Science, Bengaluru (24-28 July 2023).
14. Poster Presentation in International Winter School 2024 “*Frontiers in Materials Science*”, Organized by- Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru (02-06 December 2024).
15. Participate in webinar “*Computation| Energy and Advanced Computing in the Age of Machine Learning: From Quantum to Grid* (31 March- 1 April 2026).
16. Attended online VASP workshop “*Beyond the single particle-strongly correlated system*”, Organized by: VASP Software GmbH (13-15 April 2026).

Membership(s)

- Asian Consortium on Computational Materials Science (ACCMS) since June 2025.