Dr. Manish Kumar Mohanta

+918763522933 | mkmohanta@iitbbs.ac.in | IIT-Bhubaneswar, Odisha, India
https://manishmohanta.wordpress.com

COMPUTATIONAL MATERIALS SCIENTIST

Innovative computational materials scientist specializing in quantum materials and density functional theory. Recognized among the top 2% of scientists globally in Applied Physics by Stanford University. Expertise in electronic structure calculations, spintronics, valleytronics, and energy materials. Dedicated to advancing next-generation electronic and energy harvesting devices through advanced analytical modeling and density functional theory.

KEY EXPERTISE & CORE ACCOMPLISHMENTS

- Condensed Matter Physics
- Computational Materials Physics
- Density Functional Theory
- Quantum Materials
- Analytical Modeling
- Spintronics & Valleytronics
- Energy Materials & Devices
- Nanocluster & Catalysis

- Ranked among the top **2%** of scientists globally in Applied Physics by Stanford University in 2023, 2024 & 2025
- Published over **36** peer-reviewed articles, including Physical Review B, ACS Applied Materials & Interfaces.

PROFESSIONAL EXPERIENCE

Ramanujan Faculty November 2025-Present
Deaprtment of Physics
Indian Institute of Technology–Bhubaneswar, Odisha, India

Postdoctoral Research Fellow October 2022-October 2025
Department of Physics
Virginia Commonwealth University – Richmond, USA

Research Associate-1 April 2022- October 2022
Institute of Nano Science and Technology – Mohali, India

EDUCATION

Doctor of Philosophy in Physics **01/2017 – 06/2022**
Indian Institute of Science Education and Research (IISER) – Mohali, India
Doctoral Thesis: "**Ab initio Insights into Applied 2D Materials for Energy Harvesting and Next-generation Devices**"
Adviser: Prof. Abir De Sarkar, Institute of Nano Science and Technology – Mohali, India

Master of Science in Applied Physics **06/2014 – 05/2016**
Indian Institute of Technology (Indian School of Mines) – Dhanbad, India
CGPA: 8.9/10

Bachelor of Science in Physics **06/2011 – 05/2014**
B.J.B Autonomous College (under Utkal University) – Bhubaneswar, India
Mark: 78.8%

Intermediate **06/2009 – 05/2011**
Royal College of Science and Technology – Bhubaneswar, India
Mark: 86.83%

SKILLS & ADDITIONAL INFORMATION

Computational Skills

- VASP
- Quantum Espresso
- Gaussian
- ASE
- Phonopy
- Phono3py
- Python
- Matlab

Awards & Honors

2025	Ramanujan Faculty Fellowship – IIT-Bhubaneswar
2025	World's Top 2% Scientist Rank: **5414 –** Applied Physics, Stanford University
2024	American Physical Society (**APS**) – Division of Materials Physics (**DMP**) Post-Doctoral Travel Award
2024	World's Top 2% Scientist Rank: **3904 –** Applied Physics, Stanford University
2023	World's Top 2% Scientist Rank: **4527** – Applied Physics, Stanford University
2022	Karnataka DST Nano Science Fellowship
2017–2022	PhD fellowship/stipend sponsored by the Council of Scientific & Industrial Research (CSIR) under the Ministry of Science & Technology, Govt. of India
2016	• CSIR- JRF, AIR **94** - December • CSIR- JRF, AIR **221** – June • Joint Entrance Screening Test **(JEST)**, AIR **239** • Graduate Aptitude Test in Engineering **(GATE)**, AIR **1603**
2011–2016	INSPIRE – Scholarship for Higher Education sponsored by the Department of Science & Technology, Govt. of India

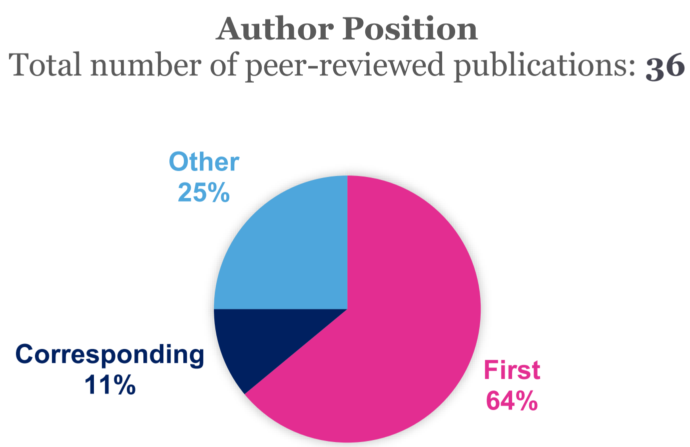
RESEARCH PUBLICATIONS

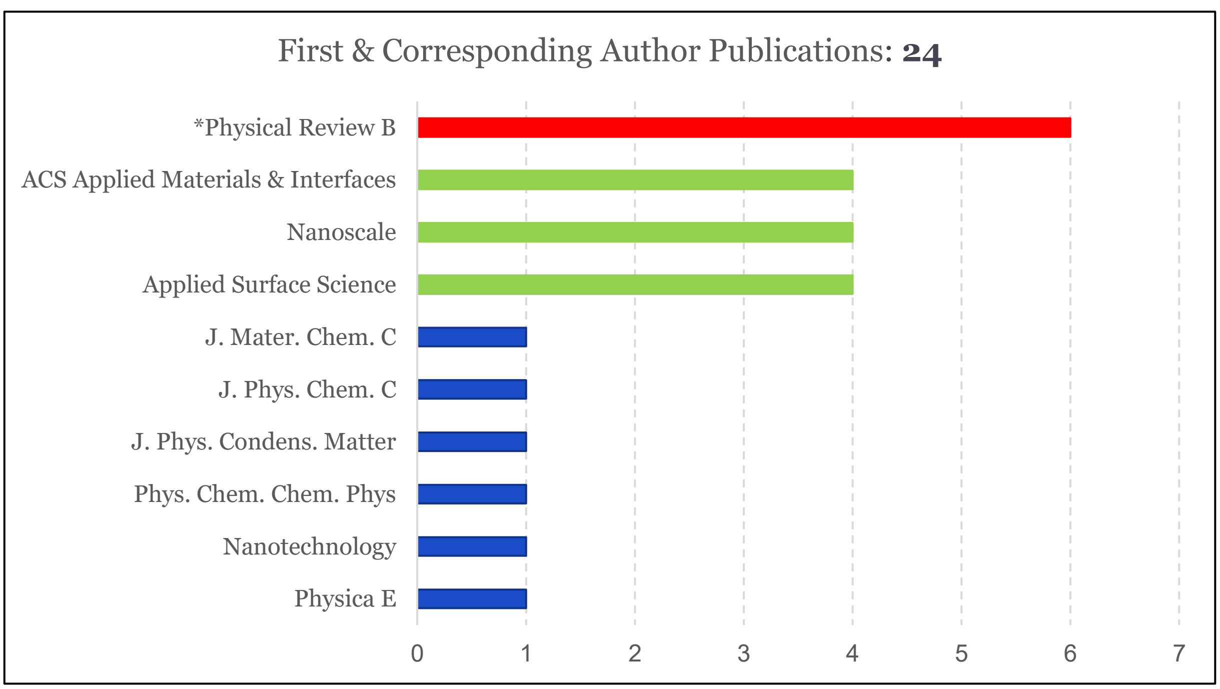
Google Scholar
https://scholar.google.com/citations?user=2QwvQDoAAAAJ&hl=en&oi=ao

ORCID
https://orcid.org/0000-0002-5476-8336

Publications Summary

- ✓ No. of citations = 1500+ (Google Scholar), h – index=**23**, i10 – index=25
- ✓ A Total of **36** papers with **24** as the **First Author**





PEER-REVIEWED PUBLICATIONS

2025		**IF**
36	**M.K. Mohanta**, P. Jena, Anomalous spin texture representation in quantum materials: Insights from density functional theory and analytical models, **Phys. Rev. B** 111 (2025) 045140. https://doi.org/10.1103/PhysRevB.111.045140.	3.2
35	**M.K. Mohanta**, P. Jena, Activation and electrochemical reduction of carbon dioxide by transition metal atom-doped copper clusters, **Nanoscale** 17 (2025) 8505–8514. https://doi.org/10.1039/D4NR03795B. **[Cover-Image]**	5.8
34	R.C. Sahoo, **M.K. Mohanta**, D. Tamudia, P. Jena, H.S.S.R. Matte, Nickel Silicate Hydroxides/Expanded Graphite as a Stable and Fast-charging Anode for the Next-generation Li-ion Batteries, **ACS Appl. Mater. Interfaces** 17 (2025) 14157–14167. https://doi.org/10.1021/acsami.4c17955.	8.5
33	S. Vishwanathan, **M.K. Mohanta**, P. Jena, H.S.S.R. Matte, Experimental and theoretical insights on interface engineered FeS/rGO as anode for fast-charging lithium- and sodium-ion batteries, **Small** 21 (2025) 2410482. https://doi.org/10.1002/smll.202410482.	13
32	M.K. Alam, **M.K. Mohanta**, D. White, J. Baker, L.S. Graves, P. Jena, I.U. Arachchige, Facile synthesis of cubic Ni1−xCrx nanoalloys and their composition-dependent electrocatalytic activity for the hydrogen evolution reaction, **Nanotechnology** 36 (2025) 225401. https://doi.org/10.1088/1361-6528/add26f.	2.9
2024		
31	**M.K. Mohanta**, P. Jena, MgTe (110) semiconductor for a magnetic-element-free nonballistic spin-field-effect transistor, **Phys. Rev. B.** 109 (2024) 085415. https://doi.org/10.1103/PhysRevB.109.085415.	3.2
30	R.C. Sahoo, P. Sahoo, **M.K. Mohanta**, P. Jena, H.S.S.R. Matte, Solution processing of spinel nickel cobaltite: Exfoliation mechanism, dispersion stability, and applications, **Inorg. Chem.** 63 (2024) 7838–7847. https://doi.org/10.1021/acs.inorgchem.4c00430.	4.3
29	**M.K. Mohanta**, P. Jena, Magnetism of Otherwise Nonmagnetic Elements: From Clusters to Monolayers, **J. Phys. Chem. C** 128 (2024) 12286–12295. https://doi.org/10.1021/acs.jpcc.4c03592.	3.3
28	**M.K. Mohanta**, P. Jena, In2Si2S3X3 (X = S, Se, Te) Janus monolayers: from magnetic element-free spin-Hall transistor to sustainable energy generation, **J. Mater. Chem. C.** 12 (2024) 1888–1896. https://doi.org/10.1039/D3TC03805J.	5.7
2023		
27	**M.K. Mohanta**, P. Jena, Symmetry-driven persistent spin texture for the two-dimensional nonsymmorphic CdTe and ZnTe crystal structures, **Phys. Rev. B.** 108 (2023) 085432. https://doi.org/10.1103/PhysRevB.108.085432.	3.2
26	**M.K. Mohanta**, F. IS, A. De Sarkar, Valley Hall effect in graphene-like SnX (X=Si, Ge) buckled monolayers with high charge carrier mobility and low lattice thermal conductivity, **Phys. Rev. B.** 107 (2023) 035429. https://doi.org/10.1103/PhysRevB.107.035429.	3.2
25	F. IS, **M.K. Mohanta**, A.D. Sarkar, Insights into selected 2D piezo Rashba semiconductors for self-powered flexible piezo spintronics: material to contact properties, **J. Phys. Condens. Matter.** 35 (2023) 253001. https://doi.org/10.1088/1361-648X/acc70f.	2.3

2022

24 **M.K. Mohanta**, H. Seksaria, A.D. Sarkar, Insights into CrS2 monolayer and n-CrS2/p-HfN2 interface for low-power digital and analog nanoelectronics, **Applied Surface Science**. 579 (2022) 152211. https://doi.org/10.1016/j.apsusc.2021.152211. 6.3

2021

23 **M.K. Mohanta**, A. Arora, A. De Sarkar, Effective modulation of ohmic contact and carrier concentration in a graphene-MgX (X=S, Se) van der Waals heterojunction with tunable band-gap opening via strain and electric field, **Phys. Rev. B.** 104 (2021) 165421. https://doi.org/10.1103/PhysRevB.104.165421. 3.2

22 **M.K. Mohanta**, F. IS, A. Kishore, A. De Sarkar, Spin-Current Modulation in Hexagonal Buckled ZnTe and CdTe Monolayers for Self-Powered Flexible-Piezo-Spintronic Devices, **ACS Appl. Mater. Interfaces.** 13 (2021) 40872–40879. https://doi.org/10.1021/acsami.1c09267. 8.3

21 **M.K. Mohanta**, A. Arora, A. De Sarkar, Conflux of tunable Rashba effect and piezoelectricity in flexible magnesium monochalcogenide monolayers for next-generation spintronic devices, **Nanoscale**. 13 (2021) 8210–8223. https://doi.org/10.1039/D1NR00149C. 5.8

20 **M.K. Mohanta**, A.D. Sarkar, 2D HfN2/graphene interface based Schottky device: Unmatched controllability in electrical contacts and carrier concentration via electrostatic gating and out-of-plane strain, **Applied Surface Science**. 540 (2021) 148389. https://doi.org/10.1016/j.apsusc.2020.148389. 6.3

19 **M.K. Mohanta**, A. Rawat, A.D. Sarkar, Atomistic manipulation of interfacial properties in HfN2/MoTe2 van der Waals heterostructure via strain and electric field for next generation multifunctional nanodevice and energy conversion, **Applied Surface Science**. 568 (2021) 150928. https://doi.org/10.1016/j.apsusc.2021.150928. 6.3

2020

18 **M.K. Mohanta**, A. De Sarkar, Coupled spin and valley polarization in monolayer HfN2 and valley-contrasting physics at the HfN2-WSe2 interface, **Phys. Rev. B.** 102 (2020) 125414. https://doi.org/10.1103/PhysRevB.102.125414. 3.2

17 **M.K. Mohanta**, A. Rawat, N. Jena, Dimple, R. Ahammed, A. De Sarkar, Interfacing Boron Monophosphide with Molybdenum Disulfide for an Ultrahigh Performance in Thermoelectrics, Two-Dimensional Excitonic Solar Cells, and Nanopiezotronics, **ACS Appl. Mater. Interfaces.** 12 (2020) 3114–3126. https://doi.org/10.1021/acsami.9b16866. 8.3

16 **M.K. Mohanta**, A.D. Sarkar, Tweaking the Physics of Interfaces between Monolayers of Buckled Cadmium Sulfide for a Superhigh Piezoelectricity, Excitonic Solar Cell Efficiency, and Thermoelectricity, **ACS Appl. Mater. Interfaces.** 12 (2020) 18123–18137. https://doi.org/10.1021/acsami.0c00864. 8.3

15 **M.K. Mohanta**, A. De Sarkar, Interfacial hybridization of Janus MoSSe and BX (X = P, As) monolayers for ultrathin excitonic solar cells, nanopiezotronics and low-power memory devices, **Nanoscale.** 12 (2020) 22645–22657. https://doi.org/10.1039/D0NR07000A. 5.8

14 **M.K. Mohanta**, I.S. Fathima, A. De Sarkar, Exceptional mechano-electronic properties in the HfN2 monolayer: a promising candidate in low-power flexible electronics, memory devices and photocatalysis, **Phys. Chem. Chem. Phys.** 22 (2020) 21275–21287. 2.9

https://doi.org/10.1039/D0CP02999H.

13 **M.K. Mohanta**, A.D. Sarkar, Giant tunability in electrical contacts and doping via inconsiderable normal electric field strength or gating for a high-performance in ultrathin field effect transistors based on 2D BX/graphene (X = P, As) van der Waals heterobilayer, **Applied Surface Science.** 526 (2020) 146749. https://doi.org/10.1016/j.apsusc.2020.146749. 6.3

12 **M.K. Mohanta**, A. Kishore, A. De Sarkar, Two-dimensional ultrathin van der Waals heterostructures of indium selenide and boron monophosphide for superfast nanoelectronics, excitonic solar cells, and digital data storage devices, **Nanotechnology.** 31 (2020) 495208. https://doi.org/10.1088/1361-6528/abaf20. 2.9

11 **M.K. Mohanta**, A. Rawat, N. Jena, R. Ahammed, A.D. Sarkar, Superhigh flexibility and out-of-plane piezoelectricity together with strong anharmonic phonon scattering induced extremely low lattice thermal conductivity in hexagonal buckled CdX (X = S, Se) monolayers, **Journal of Physics: Condensed Matter.** 32 (2020) 355301. https://doi.org/10.1088/1361-648x/ab8d73. 2.3

10 **M.K. Mohanta**, Dimple, A. Rawat, N. Jena, R. Ahammed, A.D. Sarkar, Ultra-low thermal conductivity and super-slow hot-carrier thermalization induced by a huge phononic gap in multifunctional nanoscale boron pnictides, **Physica E: Low-Dimensional Systems and Nanostructures.** 124 (2020) 114222. https://doi.org/10.1016/j.physe.2020.114222. 2.9

9 A. Medda, A. Dutta, D. Bain, **M.K. Mohanta**, A. De Sarkar, A. Patra, Electronic Structure Modulation of 2D Colloidal CdSe Nanoplatelets by Au25 Clusters for High-Performance Photodetectors, **J. Phys. Chem. C.** 124 (2020) 19793–19801. https://doi.org/10.1021/acs.jpcc.0c04774. 3.3

8 Dimple, **M.K. Mohanta**, A. Rawat, N. Jena, R. Ahammed, A.D. Sarkar, Ultra-low lattice thermal conductivity and giant phonon–electric field coupling in hafnium dichalcogenide monolayers, **Journal of Physics: Condensed Matter**. 32 (2020) 315301. https://doi.org/10.1088/1361-648x/ab7e5f. 2.3

7 R. Ahammed, A. Rawat, N. Jena, Dimple, **M.K. Mohanta**, A.D. Sarkar, ZrS3/MS2 and ZrS3/MXY (MMo, W; X, YS, Se, Te; X ≠ Y) type-II van der Waals hetero-bilayers: Prospective candidates in 2D excitonic solar cells, **Applied Surface Science**. 499 (2020) 143894. https://doi.org/10.1016/j.apsusc.2019.143894. 6.3

6 R. Ahammed, N. Jena, A. Rawat, **M.K. Mohanta**, Dimple, A. De Sarkar, Ultrahigh Out-of-Plane Piezoelectricity Meets Giant Rashba Effect in 2D Janus Monolayers and Bilayers of Group IV Transition-Metal Trichalcogenides, **J. Phys. Chem. C.** 124 (2020) 21250–21260. https://doi.org/10.1021/acs.jpcc.0c05134. 3.3

5 A. Rawat, **M.K. Mohanta**, N. Jena, Dimple, R. Ahammed, A. De Sarkar, Nanoscale Interfaces of Janus Monolayers of Transition Metal Dichalcogenides for 2D Photovoltaic and Piezoelectric Applications, **J. Phys. Chem. C.** 124 (2020) 10385–10397. https://doi.org/10.1021/acs.jpcc.0c02199. 3.3

2019

4 **M.K. Mohanta**, A. Rawat, Dimple, N. Jena, R. Ahammed, A. De Sarkar, Superhigh out-of-plane piezoelectricity, low thermal conductivity and photocatalytic abilities in ultrathin 2D van der Waals heterostructures of boron monophosphide and gallium nitride, **Nanoscale**. 11 (2019) 21880–21890. https://doi.org/10.1039/C9NR07586K. **[Editor's Choice]** 5.8

3 N. Jena, Dimple, R. Ahammed, A. Rawat, **M.K. Mohanta**, A. De Sarkar, Valley drift and valley current modulation in strained monolayer MoS_2, **Phys. Rev. B.** 100 (2019) 165413. https://doi.org/10.1103/PhysRevB.100.165413. 3.2

2 A. Rawat, R. Ahammed, Dimple, N. Jena, **M.K. Mohanta**, A. De Sarkar, Solar Energy Harvesting in Type II van der Waals Heterostructures of Semiconducting Group III Monochalcogenide Monolayers, **J. Phys. Chem. C.** 123 (2019) 12666–12675. https://doi.org/10.1021/acs.jpcc.9b03359. 3.3

2018

1 Dimple, N. Jena, A. Rawat, R. Ahammed, **M.K. Mohanta**, A.D. Sarkar, Emergence of high piezoelectricity along with robust electron mobility in Janus structures in semiconducting Group IVB dichalcogenide monolayers, **J. Mater. Chem. A.** 6 (2018) 24885–24898. https://doi.org/10.1039/C8TA08781D. 10.7

CONFERENCE PRESENTATIONS

March 2024 – American Physical Society (APS), Minnesota

1. **Title:** Symmetry-Driven Persistent Spin Texture Towards Ferromagnet-free Non-Ballistic Spintronics
   Authors: **Manish Kumar Mohanta**, Puru Jena
2. **Title:** From clusters to crystals: Magnetism of otherwise nonmagnetic elements in two-dimension
   Authors: **Manish Kumar Mohanta**, Puru Jena

PROFESSIONAL SERVICES

Peer Reviewer

- Physical Review B
- Nano Letters
- Journal of Materials Chemistry A
- Journal of Physical Chemistry Letters
- Nanoscale
- Phys. Chem. Chem. Phys
- Scientific Reports
- Materials Advances
- 2D Materials
- Journal of Materials Chemistry C
- ACS Applied Energy Materials
- ACS Omega
- Surfaces and Interfaces
- Materials Research Express

REFERENCES

1. **Prof. Puru Jena [Postdoc Supervisor]**
   Distinguished Professor, Department of Physics,
   Virginia Commonwealth University, Richmond, USA
   Email: *pjena@vcu.edu*
2. **Prof. Abir De Sarkar [PhD Supervisor]**
   Professor, Institute of Nano Science and Technology, Mohali, India
   Email: *abir@inst.ac.in*
3. **Prof. HSS Ramakrishna Matte [Experimental Collaborator]**
   Scientist-D, Centre for Nano and Soft Matter Sciences, Bengaluru, India
   Email: *matte@cens.res.in*
4. **Prof. Indika U Arachchige [Experimental Collaborator]**
   Professor, Department of Chemistry,
   Virginia Commonwealth University, Richmond, USA
   Email: *iuarachchige@vcu.edu*