Nikhil Kodali

Department of Computational and Data Sciences
Indian Institute of Science, Bengaluru 560012, India

nikhilkodali@iisc.ac.in • knikhil1995.github.io • Google Scholar • ORCID 0000-0001-6954-4880 • GitHub knikhil1995

Profile

I am a computational materials scientist with a Ph.D. from the Indian Institute of Science (defended 4 November 2026). My expertise lies in electronic-structure theory, numerical methods and high-performance computing, with a focus on both fundamental method development and materials applications. My research has contributed new mathematical formulations and scalable numerical algorithms for density functional theory, addressing key limitations in computational efficiency, robustness and scalability. These advances have extended the capabilities of first-principles simulations to larger and more complex systems, particularly those involving noncollinear magnetism and spin–orbit coupling. My research interests also extend to quantum-centric supercomputing, including hybrid quantum–classical algorithms for strongly correlated materials.

Research interests

First-principles modelling of defects and interfaces in magnetic and spintronic materials • twisted bilayers of van der Waals magnets • relativistic projector-augmented-wave methods • strongly correlated materials (Hubbard corrections, ACBN0, DMFT) • exchange–correlation functionals for noncollinear magnetism • large-scale DFT on GPU supercomputers.

Education

2021 – 2026 **M.Tech. (Research) and Ph.D., Computational and Data Sciences**
Indian Institute of Science (IISc), Bengaluru
Thesis titled *Finite-element methods and exascale algorithms for fully relativistic noncollinear pseudopotential density functional theory*, with the subtitle *From mathematical formulations to efficient computational realization and magnetic materials applications*, defended on 4 November 2026.
Advised by Prof. Phani Motamarri (MATRIX Lab). Coursework CGPA 9.2/10. Prime Minister's Research Fellow, 2023–2026.

2013 – 2017 **B.Tech. with Honours in Electrical Engineering, Minor in Physics**
Indian Institute of Technology Bombay
CGPA 8.15/10.

Fellowships and Honours

2023 – 2026 **Prime Minister's Research Fellowship (PMRF)**, Ministry of Education, Government of India (cycle 11).

2021 **CSIR Junior Research Fellowship**, with all-India rank 55 in Physical Sciences in the national eligibility test (2020).

2013 **Gold medals** in the Indian National Physics Olympiad and the Indian National Chemistry Olympiad.

2013 Selected for the Professor Harry Messel International Science School, University of Sydney.

2013 All-India rank 75, Joint Entrance Examination (Advanced).

2011 – 2013 KVPY Fellow, Department of Science and Technology, Government of India.

Research Experience

Aug 2026 – present **National Quantum Mission (NQM) Postdoctoral Fellow**, Department of Computational and Data Sciences, IISc Bengaluru

- Quantum–HPC algorithms for strongly correlated materials as part of the National Quantum Mission project SPAARQ, a consortium led by IISc with partnering institutes IIIT Hyderabad, IIT Kanpur and TCS Research (2026–2029).
- Sampling-based quantum computing algorithms for strongly correlated materials, in collaboration with IBM Research [8].

2021 – 2026 **Doctoral researcher**, MATRIX Lab, Department of Computational and Data Sciences, IISc Bengaluru, advised by Prof. Phani Motamarri

- Developed finite-element DFT methods for noncollinear magnetism and spin–orbit coupling, including atomic forces and cell stresses for structural relaxation. The methods were validated against plane-wave codes for energies, magnetic anisotropy, band structures and spin textures. They are 8–11$\times$ faster than plane-wave codes on CPUs, in minimum wall time, for semi-periodic and non-periodic systems of 5,000–7,000 electrons [3].
- Developed the R-ChFSI eigensolver and a mixed-precision, compressed-communication GPU implementation that enabled fully relativistic DFT calculations of about 80,000 electrons (a 9,114-atom twisted bilayer of $MoSe_2$) on 9,600 GPUs of the Aurora supercomputer [2, 1].
- Developing adaptive-coordinate finite-element meshes and a projector-augmented-wave formulation that improve computational efficiency for systems with hard pseudopotentials [10, 11]. Contributed to the finite-element formulation of meta-GGA functionals [9].
- All of the developments above are part of the open-source DFT-FE code, of which I am a principal developer. DFT-FE was an ACM Gordon Bell Prize finalist (Das et al., SC19) and the workhorse behind the 2023 ACM Gordon Bell Prize (Das et al., SC23).
- The methods above enabled a study of Fe vacancies in monolayer Fe_3GeTe_2, in collaboration with Prof. Biplab Sanyal (Uppsala University). The study covers site preference, local reconstruction of magnetic moments, vacancy-induced spin canting and Dzyaloshinskii–Moriya interaction, and vacancy–vacancy interaction [6].
- Developed HEXA, a standalone dense eigensolver for multi-GPU systems, for the subspace problem that limits the largest DFT calculations [7].

2017 – 2018 **Research assistant (HiWi)**, Institute for Computational Physics, University of Stuttgart (Prof. Maria Fyta)
DFT structural optimization and energy calculations for NV centres in diamond slabs and their interaction with nucleobases.

May – July 2016 **Research intern**, Nano and Hybrid Materials Group, École Polytechnique de Montréal (Prof. Oussama Moutanabbir)
DFT structural optimization and energy calculations on Si–Ge–Sn alloys, supporting the atom-probe observation of short-range order in metastable SiGeSn layers [5].

May – July 2015 **Summer research fellow**, Department of Condensed Matter Physics, S. N. Bose National Centre for Basic Sciences, Kolkata (Prof. Tanusree Saha-Dasgupta)
DFT calculations of the density of states and band gap of bulk perovskite compounds, a first step towards understanding two-dimensional electron gas formation at perovskite interfaces.

2013 – 2017 **Undergraduate projects**, IIT Bombay
B.Tech. project on the physics of $Pr_{1-x}Ca_xMnO_3$ (PCMO) resistive-memory devices (Prof. Udayan Ganguly), an instrument for contactless measurement of semiconductor

conductance (Profs. K. L. Narasimhan and B. M. Arora), and the electronic band structure of NV centres in diamond (Prof. Alok Shukla).

Publications

IF_2 and IF_5 denote the latest two-year and five-year journal impact factors (Journal Citation Reports), as listed by Web of Science and the publishers in November 2026. Quartiles are the SCImago (SJR) best quartile of the journal. The conference rank is from the CORE ranking (CORE2023). Google Scholar lists 56 citations (October 2026).

Refereed journal and conference papers

[1] **N. Kodali**, G. Panigrahi, N. Gupta, S. Gourishanker, K. Ramakrishnan, R. Panch, S. Das, V. Rao, and P. Motamarri, "Towards exascale fully relativistic pseudopotential density functional theory calculations with mixed-precision computation and compressed communication using residual-based subspace iteration," *SC26, the International Conference for High Performance Computing, Networking, Storage, and Analysis*, Chicago, 15–20 November 2026 (accepted). arXiv:2605.30128 (CORE rank A)

[2] **N. Kodali**, K. Ramakrishnan, and P. Motamarri, "Residual-based Chebyshev filtered subspace iteration for Hermitian eigenvalue problems tolerant to inexact matrix-vector products," *Computer Physics Communications* **327**, 110239 (2026). doi.org/10.1016/j.cpc.2026.110239 (IF_2 3.9, IF_5 8.4, Q1)

[3] **N. Kodali** and P. Motamarri, "Finite-element methods for noncollinear magnetism and spin-orbit coupling in real-space pseudopotential density functional theory," *Physical Review B* **111**, 195129 (2025). doi.org/10.1103/PhysRevB.111.195129 (IF_2 3.9, IF_5 3.7, Q1)

[4] G. Panigrahi†, **N. Kodali**†, D. Panda, and P. Motamarri, "Fast hardware-aware matrix-free algorithms for higher-order finite-element discretized matrix multivector products on distributed systems," *Journal of Parallel and Distributed Computing* **192**, 104925 (2024). doi.org/10.1016/j.jpdc.2024.104925 (IF_2 3.4, IF_5 3.5, Q1) (†equal contribution)

[5] S. Mukherjee, **N. Kodali**, D. Isheim, S. Wirths, J. M. Hartmann, D. Buca, D. N. Seidman, and O. Moutanabbir, "Short-range atomic ordering in nonequilibrium silicon-germanium-tin semiconductors," *Physical Review B* **95**, 161402(R) (2017). doi.org/10.1103/PhysRevB.95.161402 (IF_2 3.9, IF_5 3.7, Q1)

Manuscripts under review and in preparation

[6] **N. Kodali**, B. Sanyal, and P. Motamarri, "Vacancy-induced Dzyaloshinskii–Moriya interaction and spin canting in monolayer Fe_3GeTe_2" (under review).

[7] **N. Kodali**, "HEXA: Narrow-band reduction and banded divide and conquer for dense Hermitian eigenproblems on distributed-memory GPU systems" (under review).

[8] **N. Kodali**, S. Bhandary, D. Bhoumik, D. Vinayagamurthy, and P. Motamarri, "Quantum samples, classical accuracy: a resource-efficient strategy for sample-based quantum diagonalization" (under review).

[9] S. Nandi, K. Ramakrishnan, **N. Kodali**, G. Sai Gautam, V. Rao, and P. Motamarri, "Efficient methods for *ab initio* modeling of materials using finite-element DFT with τ-mGGA functionals" (under review).

[10] **N. Kodali** and P. Motamarri, "Adaptive-coordinate finite-element methods for efficient density functional theory calculations" (in preparation).

[11] **N. Kodali** and P. Motamarri, "Fully relativistic DFT calculations using finite-element discretization of the projector-augmented-wave method" (in preparation).

Teaching Experience

2022, 2025 — **Teaching Assistant, DS 284 Numerical Linear Algebra** (two offerings), Department of Computational and Data Sciences, Indian Institute of Science.

2023 — **Teaching Assistant, DA 219o Quantum Computing Methods**, IISc Knowledge and E-Learning Network, Indian Institute of Science.

2015, 2016 **Teaching Assistant, PH 107 Quantum Physics and Application** (two offerings), Department of Physics, Indian Institute of Technology Bombay.

Conference Presentations

March 2024 "Scalable higher-order finite-element-based methods for non-collinear magnetism and spin-orbit coupling in real-space density functional theory," contributed talk, **APS March Meeting**, Minneapolis.

Feb – Mar 2023 "Finite-element based computational methodologies for non-collinear magnetism and spin-orbit coupling in real-space density functional theory," poster, **SIAM Conference on Computational Science and Engineering**, Amsterdam.

December 2022 "An efficient hardware-aware matrix-free implementation for finite-element discretized matrix-multivector products" (with G. Panigrahi and P. Motamarri), presenting author, Student Research Symposium, **IEEE International Conference on High Performance Computing, Data, and Analytics (HiPC)**.