Lokanath Patra

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7103 Ashford Gables Dr, Dunwoody, GA, 30338

Professional Skills

Languages	Strong reading, writing, and speaking competencies in English, Hindi, and Odia (Native language).
Simulation	Density Functional Theory (DFT), ab initio and classical molecular dynamics (MD), spin-lattice dynamics (SLD), Monte Carlo, Non-Equilibrium Green Function (NEGF) simulations
Research	Solving complex lattice and magnetic structures, electronic, optical, thermal, mechanical, and magneto-electric/caloric/optical properties, orbital ordering, spontaneous electrical polarization
Programming	C, C++, FORTRAN, Python
Codes	VASP, WIEN2K, CRYSTAL17, Quantum Espresso, CALYPSO, LAMMPS, VAMPIRE, UppASD, SPR-KKR, QuantumATK.
Analysis	VESTA, Xmgrace, Origin, p4vasp, OVITO, Phonopy, XCrySDen, VMD
Misc.	Academic research, collaborative research, teaching, training, consultation, LaTeX typesetting, and publishing.

Research Experience

Sep 2024 – Cont.	**Research Engineer II,** Georgia Institute of Technology, USA.
Dec 2021 – Jul 2024	**Postdoctoral Scholar,** University of California Santa Barbara, USA.
Feb 2020 – Nov 2021	**Postdoctoral Scholar,** Michigan Technological University, USA.
Mar 2019 – Feb 2020	**Research Associate,** Indian Institute of Technology Madras, India.
Nov 2018 – Dec 2018	**Collaborative Researcher**, University of Oslo, Norway.
May 2018 – Jun 2018	**Collaborative Researcher**, University of Oslo, Norway.
Dec 2015 – Jan 2016	**Collaborative Researcher**, University of Oslo, Norway.

Education

2013 – 2019 **Ph.D. in Physics, Central University of Tamil Nadu, India** Area: Condensed Matter Physics (Computational).
Thesis title: *First Principles Modeling of Multiferroics with Giant Magnetoelectric Coupling.*

2011 – 2013 **M.Sc. in Physics, Pondicherry University, India**, Specialization: Condensed Matter Physics (Experimental)
Thesis title: *Magnetic and Dielectric Properties of $Co_{1.75}Fe_{1.25}O_4$ Spinel Ferrite Prepared by Co-Precipitation Method.*

2008 – 2011 **B.Sc. in Physics, Ravenshaw University, India**

Research Achievements

- **Observation of a giant magnetoelectric effect in perovskite oxides**
  The transition of Co^{3+} ions from high-spin to low-spin states gives rise to a giant magnetoelectric coupling effect in composites comprising $BiCoO_3$. The prominent orbital ordering of V^{4+} ions within the $PbVO_3$-based perovskite composite predominantly contributes to its elevated magnetoelectric coupling.

Research Achievements (continued)

- **Discovery of multiferroicity in bismuth-based double perovskites**
  The elucidated crystal structure of Bi_2XTiO_6 (X = Fe, Mn, Ni) double perovskites reveals the presence of $d^0 + d^n$ electron configurations, leading to the coexistence of antiferromagnetic and ferroelectric orderings..
- **Metal-insulator transition in hole- and electron-doped nickelates**
  Hole and electron-doped Ruddlesden–Popper nickelates exhibit a metal-to-insulator transition and the presence of an average valency at the nickel site.
- **Exploring the chemistry of ozonation in group IV monolayers**
  The group-IV monolayers exhibit distinct responses to ozonation, characterized by the rapid dissociation of O_3 in silicene, while graphene, germanene, and stanene demonstrate oxidation resistance. Computational simulations have been employed to elucidate the potential impact of ozonation on their electronic and photonic properties.
- **Orientation-dependent mechanical response of graphene/BN heterostructures**
  Graphene/BN hybrid van der Waals structures offer multifunctional capabilities, with mechanical strength influenced by constituent monolayer orientation. Mechanical responses vary significantly in the out-of-plane direction due to interlayer interactions but remain robust in the in-plane direction.
- **Understanding the chemical stability and mechanical response of WN nanosheets**
  The anisotropic mechanical strength in WN nanosheets can be ascribed to directional covalent bonding between W and N atoms. The opposing stabilities of W- and N-terminated surfaces in O_2 and H_2O atmospheres imply that precise growth conditions are essential to attain exceptional mechanical robustness.
- **Ternary nitride materials for solar absorbers**
  The simulated structural, optical, and electrical properties, combined with collaborative experimental measurements, highlight the potential of $MgSnN_2$ and $ZnSnN_2$ for advancements in solar absorbers and LEDs.
- **Discovery of materials for thermoelectric applications**
  Density functional theory calculations have been conducted to unveil promising thermoelectric responses in bulk half-Heusler compounds, as well as in novel AuX (X = Cu, Ag) and XO_2 (X = Pd, Pt) monolayers.
- **pH dependent adhesion of Salicylhydroxamic acid**
  Simulations were conducted on conjugated complexes involving the silica surface and the adhesive acid molecule to assess the pH dependency of SHAM–Silica interactions. The deprotonation of Salicylhydroxamic acid was identified as the underlying mechanism responsible for the emergence of novel adhesive properties.
- **Indirect exchange interaction leads to large lattice contribution to magnetocaloric entropy change**
  Spin-lattice dynamics simulations have been utilized to demonstrate that indirect exchange interactions result in extended-range spin-phonon coupling, which can engender a significant lattice contribution to magnetocaloric entropy changes.
- **Discovery of materials for magnetocaloric applications**
  Machine learning predictions, coupled with atomic spin dynamics calculations, have been utilized to explore promising magnetocaloric materials within the realm of rare earth-based compounds.

Conference Presentations (Poster and Oral)

2015 Electronic and magnetic structures of hole doped trilayer $La_4Ni_3O_8$ from first principles, International e-workshop/conference on computational condensed matter physics and materials science, Gwalior, Madhya Pradesh, October 18 – 22.

2016 Prediction of magnetoelectric behavior in Bi_2MnTiO_6, 61^{st} DAE Solid State Physics Symposium, Bhubaneswar, December 26 – 30.

2017 First-principles prediction of coexistence of magnetism and ferroelectricity in $BiFeWO_6$, International Conference on Advances in Functional Materials, Chennai, January 6 – 8.

Conference Presentations (Poster and Oral) (continued)

- Magnetoelectric properties of Pb free Bi_2FeTiO_6: A theoretical investigation, 2^{nd} International Conference on Condensed Matter & Applied Physics, Bikaner, November 24 – 25.
- Theoretical Investigation of the magnetoelectric properties of Bi_2NiTiO_6, 62^{nd} DAE Solid State Physics Symposium, Mumbai, December 26 – 30.

2018
- Design composite multiferroics with giant magnetoelectric effect, physics of strongly correlated electron systems, International conference on physics of strongly correlated electron systems, Mandi, April 02 – 04.

2020
- First-principles study of interaction of O_3 with silicene, Virtual MRS Spring/Fall Meeting & Exhibit, November 27 - December 04.

2021
- Mechanical response of graphene/BN heterostructures, American Physical Society (APS) March Meeting, Chicago, March 14 – 18.

2023
- Lattice contribution to the magnetocaloric entropy change: A spin-lattice dynamics study, American Physical Society (APS) March Meeting, Las Vegas, March 05 - 10.

2024
- Magnetocaloric behavior in 2D magnets: A dimensionality perspective, American Physical Society (APS) March Meeting, Minneapolis, March 03 - 08.

Invited Talks

2017
- *Metamagnetism induced strong magnetoelectric coupling*, Department seminar, Central University of Tamil Nadu, India, August 18.

2019
- *First-principles modeling of materials with negative thermal expansion*, Functional Materials For Energy Technology (FMET), Central University of Tamil Nadu, India, September 23-24.

2021
- *Stability and Mechanical Response of 2D Materials*, Department of Physics Colloquium, Michigan Technological University, USA, September 30.

2023
- *Stability and mechanical properties of 2D materials*, International Conference on Functional Materials, Wavoo Wajeeha Women's College of Arts and Science, India, February 28.
- *Stability and mechanical properties of 2D materials*, Simulation Center for Atomic and Nanoscale MATerials (SCANMAT), Central University of Tamil Nadu, India, March 1.
- *Stability and mechanical properties of 2D materials*, Centre for Materials Informatics (C-MaIn), Anna University, India, March 2.
- *Making a cool choice: Magnetocaloric refrigeration*, International Summer School on Materials Informatics & bio-photonics for Medical and Energy Research (InSuMMER), Anna University, India, May 29 - June 17.
- *Stability and mechanical properties of 2D materials*, Physics Scholars Symposium (PSS), Fakir Mohan University, India, July 3 - 4.

2024
- *Magnetocaloric effect in two-dimensional materials*, International Conference on Ultrasonics and Material Science for Advanced Technology (ICUMSAT), Kamaraj College and Ultrasonic Society of India (USI), CSIR-NPL, India, November 13 - 15.

Academic Experience

- Provided assistance and guidance to five postgraduate projects in computational condensed matter physics.

    1. **Anu Maria Augustine**, Predicting super hard materials based on ab initio calculations (2015).
    2. **Syam Kumar R**, Novel silicoaluminophosphate (SAPO-34) molecular sieves for selective adsorption of carbon dioxide (2016).
    3. **Mukesh Choudhary**, Designing semiconducting thermoelectric materials from metals (2016).
    4. **Y Ramya Koteswari**, Computational modeling of multiferroic solid solution with giant magnetoelectric coupling (2018).
    5. **Arjun R Krishnan**, Designing Pb-free multiferroic materials with strong coupling between the order parameters (2019).

- Conducted laboratory classes for bachelor's degree students.
- Coordinated the Computational Condensed Matter Physics Lab for M.Tech. Material Science students.
- Collaborated with my supervisor in conducting examinations and grading assignments for his coursework.
- Proficient in writing proposals for funding agencies.

Professional Affiliations and Review Activities (Review Papers: 35)

- Reviewer for Applied Surface Science
- Reviewer for RSC Advances
- Reviewer for Physical Chemistry Chemical Physics
- Reviewer for Materials
- Reviewer for Nanomaterials
- Reviewer for Molecules
- Reviewer for Crystals
- Reviewer for Journal of Physics and Chemistry of Solids
- Reviewer for Physica E: Low-dimensional Systems and Nanostructures
- Reviewer for Computational Materials Science
- Reviewer for Electronic Structure
- Reviewer for Physica Scripta
- Reviewer for Materials Research Express
- Reviewer for Surfaces and Interfaces

Leadership

- Played a key role in establishing the SCANMAT center and high-performance computing facilities at the Central University of Tamil Nadu.
- Assisted in installing and maintaining the local computer cluster in Prof. Ravindra Pandey's group at Michigan Technological University.
- Facilitated interdisciplinary communication between experimental and theoretical groups to achieve research goals at CUTN and MTU.

Leadership (continued)

- Collaborated with experimental research teams to provide computational support and data analysis.
- One of the organizers for three national and two international conferences at CUTN
- Member of the international advisory committee for the *International Conference on Ultrasonics and Materials Science for Advanced Technology* (*ICUMSAT 2024*), organized by Kamaraj College, Thoothukudi, Tamil Nadu and Ultrasonic society of India (USI), New Delhi.
- Coordinator for the Computational Condensed Matter Physics Lab for M.Tech. Material Science students at CUTN.
- Mentored undergraduate and graduate students for research.

Research Publications

Journal Articles

1 Choudhary, M. K., Rawat, A., **Patra**, **L.** & Pandey, R. First-principles study of Chlorination of 2D monolayer. Manuscript under review (2025).

2 Mondal, S., Rajan, K. D., **Patra**, **L.**, Rathinam, M. & Ganesh, V. Sulfur Vacancy-Induced Enhancement of Piezocatalytic H_2 Production in MoS_2. *Small,* 2411828 (2025).

3 Munisha, B., **Patra**, **L.**, Nanda, J. & Mondal, S. Insights into the electronic, magnetic structure, and photocatalytic activity of Y_2CuMnO_6 double perovskite. *RSC Advances* **15,** 3110–3121 (2025).

4 Das, S. K., **Patra**, **L.**, Samal, P. & Sahoo, P. K. Strain-induced enhanced performance in 2D C_2N/MoS_2 Heterostructures for Photocatalytic water splitting: A meta-GGA study. *ACS Applied Electronic Materials* **6,** 1415–1423 (2024).

5 Das, S. K., **Patra**, **L.**, Samal, P. & Sahoo, P. K. Unveiling the reactivity of oxygen and ozone on C_2N monolayer. *Physica Status Solidi – Rapid Research Letters,* 2400148 (2024).

6 Kaur, B., Heena, Khandy, S. A., Ahmad, S. R., Albaqami, M. D., Srinivasan, M., **Patra**, **L.**, Dhiman, S. & Kaur, K. Thermoelectric properties of 2D Sn_2SSe monolayer. *Advanced Quantum Technologies* **7,** 2300357 (2024).

7 Mohapatra, S. R., **Patra**, **L.**, Pati, A., Singh, A. K., Panda, J. & Mohanty, H. S. (Contributed equally as first author), Insight into structural, electronic and magnetic properties of Gd-substituted $Bi_2Fe_4O_9$ multiferroic by experimental and theoretical approach. *ECS Journal of Solid State Science and Technology* **13,** 113010 (2024).

8 Mondal, S., **Patra**, **L.**, Ilanchezhiyan, P., Bernaurdshaw, N., Pandey, R. & Ganesh, V. In-situ growth of $CuBi_2O_4/Bi_2O_3$ Z-scheme heterostructures for bifunctional photocatalytic application. *Langmuir* **40,** 12954 (2024).

9 **Patra**, **L.**, Quan, Y. & Liao, B. Impact of dimensionality on the magnetocaloric effect in two-dimensional magnets. *Journal of Applied Physics* **136,** 024301 (2024).

10 Rawat, A., **Patra**, **L.**, Pandey, R. & Karna, S. P. First-principles study of the oxidation susceptibility of WS_2, WSe_2, and WTe_2 monolayers. *Nanoscale* **16,** 7437–7442 (2024).

11 Remya, U. D., Arun, K., Swathi, S., Athul, R. S., **Patra**, **L.**, Dzubinska, A., Reiffers, M., Pandey, R. & Nagalakshmi, R. Magnetic and Magnetocaloric Properties of $Tb_{1.4}Dy_{0.6}In$ Compound. *Journal of Alloys and Compounds* **976,** 173111 (2024).

12 Srinivasan, M., Sivasamy, R., Kaur, K., Sindhu, K. N. H., Khandy, S. A. & **Patra**, **L.** Structural Preferences of Metal Chalcogenide based Nanothreads (MX; M=Au, Ag; X=S, Se): A Computational Study. *ChemistrySelect* **9,** e202401201 (2024).

13 Yuan, J., Yang, R., **Patra**, **L.** & Liao, B. (Contributed equally as first author), Enhancing magnetocaloric material discovery: A machine learning approach using an autogenerated database by large language models. *AIP Advances* **14,** 085125 (2024).

14 Zhang, F., **Patra**, **L.**, Chen, Y., Ouyang, W., Sarte, P., Adajian, S., Zuo, X., Yang, R., Luo, T. & Liao, B. Room-temperature magnetic thermal switching by suppressing phonon-magnon scattering. *Phys. Rev. B* **109,** 184411 (2024).

15 Chinnakutti, K. K., Kirubaharan, A. K., **Patra**, **L.**, Pandey, R., Theerthagiri, J., Vengatesh, P., Salammal, S. T., Paramasivam, N., Sambandam, A., Kasemchainan, J. & Choi, M. Y. Modulating the combinatorial target power of $MgSnN_2$ via RF magnetron sputtering for enhanced optoelectronic performance: Mechanistic insights from DFT studies. *ACS Applied Materials & Interfaces* **15,** 14546–14556 (2023).

16 Munisha, B., **Patra**, **L.**, Nanda, J., Pandey, R. & Brahma, S. S. $CeMnO_3$ nanoparticle-decorated g-C_3N_4 nanosheets as Z-Scheme heterostructures for efficient photocatalytic degradation of dyes. *ACS Applied Nano Materials* **6,** 20539–20555 (2023).

17 **Patra**, **L.** & Liao, B. Indirect exchange interaction leads to large lattice contribution to magnetocaloric entropy change. *Physics Review Letters* **131,** 066703 (2023).

18 Wang, K., **Patra**, **L.**, Liu, B., Zhang, Z., Pandey, R. & Lee, B. P. Salicylhydroxamic acid as a novel switchable adhesive molecule. *Chemistry of Materials* **35,** 5322–5330 (2023).

19 Wani, A. F., Khandy, S. A., **Patra**, **L.**, Srinivasan, M., Singh, J., Ali, A. M., Islam, I., Dhiman, S. & Kaur, K. Intrinsic and strain dependent ultralow thermal conductivity in novel AuX (X = Cu, Ag) monolayers for outstanding thermoelectric applications. *Physical Chemistry Chemical Physics* **25,** 21736–21747 (2023).

20 Wani, A. F., **Patra**, **L.**, Srinivasan, M., Singh, J., Abdelmohsen, S. A., Alanazi, M. M., Dhiman, S. & Kaur, K. XO_2 (X = Pd, Pt) monolayers: A promising thermoelectric materials. *Advanced Theory and Simulations* **6,** 2300158 (2023).

21 Kumar Chinnakutti, K., **Patra**, **L.**, Panneerselvam, V., Govindarajan, D., Kheawhom, S., Theerthagiri, J., Yu, Y., Salammal, S. T. & Choi, M. Y. Lithium inserted $ZnSnN_2$ thin films for solar absorber: n to p-type conversion. *Materials Today Chemistry* **25,** 100957 (2022).

22 **Patra**, **L.**, Mallick, G., Pandey, R. & Karna, S. P. Surface stability of WN ultrathin films under O2 and H2O exposure: A first-principles study. *Applied Surface Science* **588,** 152940 (2022).

23 **Patra**, **L.** & Pandey, R. Mechanical properties of 2D materials: A review on molecular dynamics based nanoindentation simulations. *Materials Today Communications* **31,** 103623 (2022).

24 Rani, B., Wani, A. F., Khandy, S. A., Sharopov, U. B., **Patra**, **L.**, Kaur, K. & Dhiman, S. Pursuit of stability, electronic and thermoelectric properties of novel PdVGa half heusler compound. *Solid State Communications* **351,** 114796 (2022).

25 Rani, B., Wani, A. F., Sharopov, U. B., **Patra**, **L.**, Singh, J., Ali, A. M., Abd El-Rehim, A., Khandy, S. A., Dhiman, S. & Kaur, K. Electronic structure-, phonon spectrum-, and effective mass-related thermoelectric properties of PdXSn (X= Zr, Hf) half Heuslers. *Molecules* **27,** 6567 (2022).

26 Bano, A., **Patra**, **L.** & Pandey, R. Stability and electronic properties of the graphene-supported FeO nanostructures including clusters and monolayer. *Applied Surface Science* **569,** 150976 (2021).

27 Jana, S., Bhat, S. G., Behera, B., **Patra**, **L.**, Kumar, P. A., Nanda, B. & Samal, D. Evidence for weak-antilocalization–weak-localization crossover and metal-insulator transition in $CaCu_3Ru_4O_{12}$ thin films. *Europhysics Letters* **133,** 17005 (2021).

28 **Patra**, **L.**, Mallick, G. & Pandey, R. Orientation-dependent electronic and mechanical properties of tungsten nitride nanosheets: Implications for flexible devices. *ACS Applied Nano Materials* **4,** 13771–13777 (2021).

29 **Patra**, **L.**, Mallick, G., Sachdeva, G., Shock, C. & Pandey, R. Orientation-dependent mechanical response of graphene/BN hybrid nanostructures. *Nanotechnology* **32,** 235703 (2021).

30 **Patra**, **L.**, Sachdeva, G., Pandey, R. & Karna, S. P. Ozonation of group-IV elemental monolayers: A first-principles study. *ACS Omega* **6,** 19546–19552 (2021).

31 Periyasamy, M., **Patra**, **L.**, Fjellvåg, Ø. S., Ravindran, P., Sørby, M. H., Kumar, S., Sjåstad, A. O. & Fjellvåg, H. Effect of electron doping on the crystal structure and physical properties of an n = 3 Ruddlesden–Popper compound $La_4Ni_3O_{10}$. *ACS Applied Electronic Materials* **3,** 2671–2684 (2021).

32 Pan, Z., Chen, J., Yu, R., **Patra**, **L.**, Ravindran, P., Sanson, A., Milazzo, R., Carnera, A., Hu, L., Wang, L., Yamamoto, H., Ren, Y., Huang, Q., Sakai, Y., Nishikubo, T., Ogata, T., Fan, X., Li, Y., Li, G., Hojo, H., Azuma, M. & Xing, X. Large negative thermal expansion induced by synergistic effects of ferroelectrostriction and spin crossover in $PbTiO_3$-based perovskites. *Chemistry of Materials* **31,** 1296–1303 (2019).

33 **Patra**, **L.**, Vidya, R., Fjellvåg, H. & Ravindran, P. Giant magnetoelectric coupling in multiferroic $PbTi_{1-x}V_xO_3$ from density functional calculations. *ACS Omega* **4,** 16743–16755 (2019).

34 **Patra**, **L.**, Pan, Z., Chen, J., Azuma, M. & Ravindran, P. Metamagnetism stabilized giant magnetoelectric coupling in ferroelectric $x BaTiO_3 - (1-x)BiCoO_3$ solid solution. *Physical Chemistry Chemical Physics* **20,** 7021–7032 (2018).

35 Kishore, M. A., Okamoto, H., **Patra**, **L.**, Vidya, R., Sjåstad, A. O., Fjellvåg, H. & Ravindran, P. Theoretical and experimental investigation on structural, electronic and magnetic properties of layered Mn_5O_8. *Physical Chemistry Chemical Physics* **18,** 27885–27896 (2016).

36 **Patra**, **L.**, Kishore, M. A., Vidya, R., Sjåstad, A. O., Fjellvåg, H. & Ravindran, P. Electronic and magnetic structures of hole doped trilayer $La_{4-x}Sr_xNi_3O_8$ from first-principles calculations. *Inorganic Chemistry* **55,** 11898–11907 (2016).

Conference Proceedings

1 Augustine, A. M., Sudarsanan, V., **Patra**, **L.**, Kavitha, M. & Ravindran, P. *Li-rich $Li_6Mn_xFe_{(1-x)}S_4$ as cathode material for Li-ion battery* **in** *AIP Conference Proceedings* **2115** (2019).

2 **Patra**, **L.** & Ravindran, P. *Magnetoelectric properties of Pb free Bi_2FeTiO_6: A theoretical investigation* **in** *AIP Conference Proceedings* **1953** (2018).

3 **Patra**, **L.** & Ravindran, P. *Theoretical investigation of the magnetoelectric properties of Bi_2NiTiO_6* **in** *AIP Conference Proceedings* **1942** (2018).

4 **Patra**, **L.** & Ravindran, P. *Prediction of magnetoelectric behavior in Bi_2MnTiO_6* **in** *AIP Conference Proceedings* **1832** (2017).

Books and Chapters

1 Mehak, N., Wani, A. F., Rani, B., Sharopov, U. B., Singh, J., Khandy, S. A., **Patra**, **L.**, Dhiman, S. & Kaur, K. *Thermoelectric Properties of Perovskites Materials* (Nova Science Publishres, 2024).

References

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