

Dr.E.NARSIMHA RAO



CONTACT INFORMATION

Current Address :

Department of Physics, Informatics and Mathematics
Università degli Studi di Modena e Reggio Emilia
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STATEMENT OF PROFESSIONAL OBJECTIVE

To leverage my expertise in high-throughput screening, first-principles simulations, and machine learning to advance research on 2D materials, heterostructures, topological insulators, SHG, high-energy materials, and molecular systems. My focus includes impactful applications in cutting-edge technologies. With a strong foundation in programming, data analysis, and condensed matter physics, I am keen to expand my expertise in data science, driving innovation in both scientific research and industry. My goal is to contribute to cutting-edge advancements in materials science while broadening my impact through data-driven and computational solutions.

RESEARCH INTERESTS

High-throughput screening, machine learning models, Python programming, 2D materials and heterostructures, topological materials, noncentrosymmetric materials, strain and pressure engineering, spin-orbit coupling, noncollinear magnetism, data-driven computational solutions.

RESEARCH IDS

Google Scholar giRjnMAAAAJ
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ORCID 0000-0002-0928-6426
Scopus 56035742100
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TECHNICAL SKILLS

Programming and Scripting Languages: Quantum Espresso, Wannier90, Wanniertools, WannierBerri, high-throughput screening, Machine Learning with Python, WIEN2K, EXCITING, MATERIAL STUDIO (CASTEP), GAUSSIAN-09, Multiwfn, VASP etc.

Tools: Phonopy, Xmgrace, Origin, Octave, Latex, Gnuplot, Gaussview, VESTA etc.

Theoretical: Physics of Semiconductors, Solid State Physics, Quantum Mechanics, Density Functional Theory, Quantum Chemistry, Non-Linear Optics, High Energy Materials;

Interpersonal: Leadership, Collaboration, Handling Pressure and Problem-Solving skills.

National Exams Qualified: JEST(Physics), 2010, Roll No3201010057, Percentile-84.99.

PROFESSIONAL EMPLOYMENT

University of Modena and Reggio Emilia

October 2024 – Present

via Campi 213/a, 41125 Modena, Italy

Post-Doctoral Fellow

Project Title: “High-throughput characterization of two-dimensional materials and heterostructures from first principles”

Supervisor: Prof. Marco Gibertini

University of Hyderabad (UoH)

June 2020 – February 2024

Hyderabad, Telangana, India

Project-Scientist

Project Title: “The development of a theoretical model for quantitative estimation of impact sensitivity of high energy materials (HEM) and co-crystals”
Supervisor: Prof. M. Durga Prasad

University of Hyderabad (UoH) June 2019 – June 2020
Hyderabad, Telangana, India
Post-Doctoral Fellow
Project Title: “Structure-property-sensitivity correlation studies of HEM molecules, clusters, and solids”
Supervisor: Prof. M. Durga Prasad

University of Hyderabad (UoH) October 2018 – April 2019
Hyderabad, Telangana, India
Project Staff
Project Title: “Structure-property-sensitivity correlation studies of noncentrosymmetric HEM’s for NLO applications”
Supervisor: Prof. G.S. Vaitheeswaran

University of Hyderabad (UoH), Hyderabad, Telangana, India.
Senior Research Fellow (SRF) April 2014 – August 2018

University of Hyderabad (UoH), Hyderabad, Telangana, India.
Junior Research Fellow (JRF) August 2010 – March 2014

EDUCATION

University of Hyderabad (UoH) March 2019
Hyderabad, Telangana, India
Doctor of Philosophy (Ph.D. in Theoretical Condensed Matter Physics)
Thesis Submitted on: August, 2018.
Coursework: Electronic Structure Theory, Laser Primer, Concepts of Material Science, Research Methodology, Matlab, Combustion.
Thesis Title: “Structure-property correlation studies of Carbonate Fluorides and Metal-Organic Energetic solids”
Supervisor: Prof. G.S. Vaitheeswaran, Prof. S.P.Tewari

Kakatiya University, Telangana, India May 2008
Master of Science (M.Sc. Physics with Electronics specialization) (Score : 64.0%)
Main Subjects: Mathematical Physics, Classical Mechanics, Solid State Physics, Statistical Mechanics, Nuclear Physics, Quantum Mechanics, Computational Methods & Programming , Electro Magnetic Theory and Optics, Molecular and Resonance Spectroscopy, Electronics, Electronic Devices and Circuits, Electronics Microprocessors, Electronic Communication Systems

Kakatiya University, Telangana, India June 2005
Batchelor of Science (B.Sc. Computer Science) (Score : 58.0%)
Subjects: Mathematics, Physics, Computer Science (SQL, DBMS, C, C++), Numerical Analysis, Operating Systems

Board of Intermediate Education, AP, India March 2002
XIIth (Score : 72.6%)

Board of Secondary Education, AP, India March 2000
Xth (Score : 59%)

PERSONAL DATA

Date of birth : July 05, 1985

Birth Place: Pinapaka VI. Thallada MD, Khammam Dist, Telangana, India 507165

Sex : Male

citizenship : Indian

Civil status : Married, Two Children (2019, 2024)

Languages Known : English, Telugu, Hindi.

Permanent Address : S/O Elaprolu Ramamurthy, H-No:4-25, Near Satyanarayana Swami Temple, Main Road, Pinapaka (Village, Post), Thallada (Mandal), Khammam (Dist), Telangana, India. 507165. Phone: +919959594410

PERSONAL ACHIEVEMENTS

I received the Best Paper Award for a poster titled "Orientation Dependence of Mechanical Sensitivity of -5-nitro-2,4-dihydro-3H-1,2,4-triazol-3-one (NTO): A High-Pressure Study" by E. Narsimha Rao and V. Kameswara Rao, presented at the "13th International High Energy Materials Conference and Exhibits - 2022" held at TBRL, Chandigarh, Delhi from May 26 to May 28, 2022.

<https://herald.uohyd.ac.in/best-paper-presentation-award-at-hemce-2022-for-dr-elaprolu-narsimha-rao/>

PUBLICATIONS

- **Elaprolu Narsimha Rao**, S. Appalakondaiah, Yedukondalu Neelam, Ganapathy Vaitheeswaran, "Structural, electronic and optical properties of novel carbonate fluorides ABCO₃F (A=K, Rb, Cs; B=Ca, Sr)", Journal of Solid State Chemistry, 2014, 212 (0), 171-179. (IF:2.299). DOI: 10.1016/j.jssc.2014.01.015
- **E. Narsimha Rao**, G. Vaitheeswaran, A. H. Reshak, S. Auluck, "Effect of lead and cesium on the mechanical, vibrational and thermodynamic properties of hexagonal fluorocarbonates: A comparative first principles study", RSC Advances, 2016, 6, 99885-99897. (IF:3.108). DOI: 10.1039/C6RA19168B
- **E. Narsimha Rao**, A. H. Reshak, S. Auluck, G. Vaitheeswaran, "Role of spin-orbit interaction on the nonlinear optical response of CsPbCO₃F using DFT", Physical Chemistry Chemical Physics, 2017, 19, 31255-31266. (IF:4.123). DOI: 10.1039/C7CP06110H
- **Elaprolu Narsimha Rao**, Ganapathy Vaitheeswaran, "Structure-property correlation studies of Potassium 4,4-Bis(dinitromethyl)-3,3-azofurazanate: A Noncentrosymmetric Primary Explosive", The Journal of Physical Chemistry C, 2019, 123 (15), 10034-10050. (IF:4.484). DOI: 10.1021/acs.jpcc.8b11157
- Ganesh Damarla#, **Elaprolu Narsimha Rao**#, M. Venkatesh, Nagarjuna Kommu, G. Vaitheeswaran, Akhila K. Sahoo, A.K. Chaudhary, "A Time Domain Terahertz Spectroscopy and DFT studies of Nitro/Nitrogen Rich Aryl-Tetrazole Derivatives", #Equal contribution, ACS Omega, 2020, 5 (6), 2541-2551. (IF:2.584). DOI: 10.1021/acsomega.9b03678
- Atahar Parveen, **Elaprolu Narsimha Rao**, Adivaiah Bushnagar, P. Anees, Ganapathy Vaitheeswaran, "Topological behavior of ternary non-symmorphic crystals KZnX (X = P, As, Sb) under pressure and strain: A first principles study", Physical Chemistry Chemical Physics, 2018, 20, 5084-5102. (IF:4.123). DOI: 10.1039/C7CP07857D
- B. Adivaiah, **E. Narsimha Rao**, A. Parveen, G. Vaitheeswaran, "Lattice dynamics and Thermodynamic properties of alkaline-earth metal nitrates M(NO₃)₂ (M= Sr, Ba): A First principles study", Journal of Physics and Chemistry of Solids, 2018, 122, 268-277. (IF:2.048). DOI: 10.1016/j.jpccs.2018.06.003
- J. Prathap Kumar, **E. Narsimha Rao**, G. Vaitheeswaran, "Structure-Optical isotropy correlations of Alkali Metal Perchlorates MClO₄ (M = Li, Na, K, Rb, Cs)", Journal of Physics: Condensed Matter, 2018, 30, 475402 (1-16). (IF:2.745). DOI: 10.1088/1361-648X/aade1b

- S. Mondal, J. Prathap Kumar, **E. Narsimha Rao**, G. Vaitheeswaran, "Structure-property correlation studies of Bis(nitrofurazano)furazan (BNFF-1): A Density functional theory study", AIP Conference Proceedings, 2019, 2115, 030391. <https://doi.org/10.1063/1.5113230>. DOI: 10.1063/1.5113230
- B. Adivaiah, **E. Narsimha Rao**, G. Vaitheeswaran, "Structure-Property Correlation Studies of Alkaline-earth Metal-Azides $M(N_3)_2$ ($M = Sr, Ba$)", Journal of Physics: Condensed Matter, 2019, 31(47):475402. (IF:2.745). DOI: 10.1088/1361-648X/ab36a0
- T. Atahar Parveen, **E. Narsimha Rao**, B. Adivaiah, G. Vaitheeswaran, "ROLE OF SPIN-ORBIT INTERACTION ON ELECTRONIC PROPERTIES OF Cu BASED TERNARY ZINTL PHASES", 7th Annual International Conference on Emerging Research Areas (AICERA), 2017, 1-20.
- **Elaprolu Narsimha Rao***, V. Kameswara Rao*, "Pressure, Directional Dependent Mechanical Anisotropies and Phase Transition Studies of -5-nitro-2,4-dihydro-3H-1,2,4-triazol-3-one (NTO) and 2,4,6-triamino-1,3,5-trinitrobenzene (TATB)", Journal of Physics: Condensed Matter, 2022. DOI: 10.1088/1361-648X/aca199 (IF:2.745)

CONFERENCES PRESENTATIONS

- Presented a poster entitled "Orientation Dependence of Mechanical Sensitivity of -5-nitro-2,4-dihydro-3H-1,2,4-triazol-3-one (NTO): A High-Pressure Study" by **E. Narsimha Rao**, V. Kameswara Rao at the "13th International High Energy Materials Conference and Exhibits -2022" held at TBRL, Chandigarh, Delhi during May 26-28, 2022.
- Presented a poster entitled "Reconstruction of Nitrotriazolone (NTO) Crystal Packing Based on Intermolecular Interactions" by **E. Narsimha Rao**, V. Kameswara Rao, M. Durga Prasad at DAE Symposium on Current Trends in Theoretical Chemistry (CTTC-2020), September 23-25, 2021.
- Presented a poster entitled "Structure-property correlation studies of Bis(nitrofurazano)furazan (BNFF-1): A Density functional theory study" by S. Mondal, J. Prathap Kumar, **E. Narsimha Rao**, G. Vaitheeswaran, at the 63rd DAE-SSPS-2018 symposium, December 18-22, held at Guru Jambheshwar University Science and Technology, Haryana, India.
- Presented a poster entitled "Lattice dynamics of cubic alkaline-earth metal nitrates $M(NO_3)_2$ ($M = Sr, Ba$): A first principles study" by B. Adivaiah, **E. Narsimha Rao**, T. Atahar Parveen, G. Vaitheeswaran during the 11th International High Energy Materials Conference and Exhibits (HEMCE-2017) held at HEMRL, Pune during November 2017.
- Presented a poster entitled "First Principle Study of Carbonate Fluorides $ABCO_3F$ ($A = K, Rb, Cs; B = Ca, Sr$): A New Class of NLO Materials" by **E. Narsimha Rao**, G. Vaitheeswaran during the workshop entitled "Development of Binders and Plasticizers for Energetic Applications" held at ACRHEM, University of Hyderabad on December 15th, 2017.
- Presented a poster entitled "First Principle Study of Carbonate Fluorides $ABCO_3F$ ($A = K, Rb, Cs; B = Ca, Sr$): A New Class of NLO Materials" by **E. Narsimha Rao**, G. Vaitheeswaran during the Winter School held at JNCASR, Bangalore, during January 2015, India.

SCIENTIFIC ACTIVITIES & WORKSHOPS ATTENDED

- Participated in the 13th International High Energy Materials Conference Exhibits-2022 organized by High Energy Materials Society of India Chandigarh-Delhi Chapter in association with Terminal Ballistics Research Laboratory (TBRL), Chandigarh at TBRL Ranges, Ramgarh, Panchkula, Haryana, India during May 26-28, 2022.

- Participated in DAE Symposium on Current Trends in Theoretical Chemistry (CTTC-2020), September 23-25, 2021.
- Participated in Science Academies Sponsored Refresher Course on “Computational Chemistry”, held from January 27, 2020 to February 11, 2021.
- Participated in Winter School on “Computational Chemistry and Biology” during December 09-27, 2019.
- Participated in the workshop entitled “(ML4SCI-2019) on “Machine Learning of Science” during November 29 to December 1, 2019, at IIIT Hyderabad.
- Participated in the workshop entitled “Advances in Optics and Photonics” scheduled from March 17-23, 2019 organized at UGC-Networking Resource Centre, School of Physics, University of Hyderabad, Hyderabad.
- Participated in the workshop on “Development of Binders and Plasticizers for Energetic Applications” held at ACRHEM, University of Hyderabad on December 15, 2017.
- Participated in the “5th Indian Theoretical Chemistry Symposium” held at University of Hyderabad during December 2016.
- Participated in the “10th International High Energy Materials Conference and Exhibits (HEMCE-2016)” held at University of Hyderabad during February 2016.
- Participated in a one-day symposium on “Aneesur Rahman Day Lectures on Molecular Simulations” on August 24, 2016, held at ACRHEM, University of Hyderabad.
- Participated in a one-day symposium on “Aneesur Rahman Day Lectures on Molecular Simulations” on August 24, 2015, held at ACRHEM, University of Hyderabad.
- Participated in the Winter School on “Materials and Processes for Applications in Energy and Environment” during January 2015 at JNCASR, Bangalore.
- Participated in a one-day symposium on “Aneesur Rahman Day Lectures on Molecular Simulations” on August 24, 2014, held at ACRHEM, University of Hyderabad.
- Participated in the SERB School on “Materials Modeling and Simulation across Length Scale” at the Physics Department, University of Mumbai during December 2013.
- Participated in a one-day symposium on “Aneesur Rahman Day: Molecular Simulations” on August 24, 2013, held at ACRHEM, University of Hyderabad.
- Participated in the conference on “Electronic Structure Approaches to Atoms, Molecules, Clusters and Solids” held at ACRHEM, University of Hyderabad, during January 2013.
- Participated in the MaX School: Materials and Molecular Modelling with QUANTUM ESPRESSO (QE-Max-2024) course, organized by the MaX CoE, NCC Austria, NCC Czechia, NCC Hungary, NCC Poland, NCC Slovakia, and NCC Slovenia. The course was conducted online from June 19-21, 2024.
- Attended the virtual conference “MLM4MS: Machine Learning Modalities for Materials Science,” held from May 13 to 17, 2024. The conference was hosted by the Jožef Stefan Institute in Ljubljana, Slovenia.

- Attended “CS50AI: CS50’s Introduction to Artificial Intelligence with Python,” a course of study offered by HarvardX, an online learning initiative of Harvard University, Cambridge, Massachusetts, in August 2024.

RESEARCH SUMMARY

My research has been deeply rooted in the principles of quantum mechanics, focusing on the electronic properties of advanced materials through various computational methods. During my Ph.D., I employed density functional theory (DFT) to study the “Structure-property correlation of Carbonate Fluorides and Metal-Organic Energetic Solids” for Terahertz detection and nonlinear optical (NLO) applications. DFT allowed me to model the many-electron Hamiltonian effectively, enabling the exploration of how electronic wavefunctions contribute to phenomena such as second harmonic generation (SHG). This work was instrumental in designing materials with enhanced optical properties, crucial for applications like explosive detection and medical imaging. In my first postdoctoral position, I transitioned to more sophisticated, wavefunction-based quantum chemistry methods, which provided a more accurate treatment of electron correlation. This approach was essential for studying high-energy materials (HEMs) and understanding their impact sensitivity. By modeling the electronic structure of HEMs with greater precision, I uncovered how subtle changes in electron correlation can affect material stability and reactivity, offering critical insights for the design of safer and more effective materials for defense applications.

Currently, my research focuses on the modern theory of Berry phases and Berry curvature, which are key to understanding the geometric properties of electronic wavefunctions in solids. This work builds on my previous studies by exploring how topological aspects of the electronic structure influence macroscopic properties like anomalous Hall conductivity (AHC). The Berry phase provides insights into material properties not captured by traditional methods, making it particularly relevant for designing materials with unique electronic and magnetic properties, essential for spintronics and quantum computing. Moving forward, I aim to integrate these quantum mechanical approaches with high-throughput screening (HTS) and machine learning to accelerate the discovery of materials with novel topological and electronic characteristics. This comprehensive framework will enable the rapid exploration of 2D materials and heterostructures, guiding the design of materials with tailored properties for applications in optoelectronics, energy storage, and defense technologies. By bridging the gap between theoretical predictions and practical applications, my work seeks to drive the next generation of technological advancements.

REFERENCES

Prof. Marco Gibertini
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University of Hyderabad (UoH)
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Prof. Soma Venugopal Rao
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