Manas Sharma

PhD (Physics)

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Research Interests

My passion lies in **developing codes and methods** for modeling various phenonmena and processes in materials science such as **light-matter interactions**, **adsorbate-substrate interactions**, and **thin film deposition**. During my Ph.D., I focused on improving and accelerating **quantum embedding techniques** for molecular and periodic systems. I implemented **density functional theory (DFT)-based embedding** methods and coupled them with **real-time time-dependent DFT** (RT-TDDFT) and **wavefunction theory** (WFT) methods. Notably, I calculated excitation energies of solvated molecules and adsorption energies of molecule-periodic systems using WFT-in-DFT, achieving high accuracy at a fraction of the computational cost. My work also extended to **molecule-in-periodic embedding** and **high harmonic generation** via RT-TDDFT.
In my postdoctoral research, I have diversified into **machine-learned interatomic potentials** (MLIPs), particularly **graph neural network** (GNN)-based potentials, to study **chemical vapor deposition** (CVD) or **physical vapor deposition** (PVD) of thin films on substrates. To explore deposition processes at the atomic scale, I use DFT calculations and **nudged elastic band** (NEB) methods to study **reaction pathways** and **energy barriers**, as well as **ab initio molecular dynamics** (AIMD) to study dynamic evolution. Using the data from these simulations, I develop MLIPs trained on high-fidelity data and also leverage **foundation models** to extend their applicability.
Beyond simulations, I have a keen interest in **developing computational tools** for researchers. I have built a performant DFT code as well as a neural network library from scratch, optimized for parallelization and GPU acceleration. Additionally, I have experience creating GUIs for materials modeling, visualization, and input file generation.
Outside research, I enjoy creating YouTube tutorials, web & Android apps, and computer software/libraries for researchers and students.

About me

I am a postdoctoral researcher in the Chemical Engineering Department at the Indian Institute of Science (IISc), jointly advised by Prof. Ananth Govind Rajan and Prof. Sudeep Punnathanam. My current work focuses on developing **graph neural network (GNN)-based interatomic potentials** for simulating thin-film growth processes such as CVD and PVD, alongside performing density functional theory (DFT) and nudged elastic band (NEB) calculations to study atomic-scale reaction mechanisms. I also design and optimize efficient computational workflows and tools for large-scale atomistic simulations.

Previously, I obtained my Ph.D. (in Physics) from Friedrich Schiller University Jena (FSU) in Germany, with the highest distinction of *summa cum laude*, under the supervision of Prof. Dr. Marek Sierka. During my Ph.D., I developed and implemented advanced **DFT-based quantum embedding** methods coupled with **wavefunction** and **real-time TDDFT** approaches, contributing new capabilities to the TURBOMOLE quantum chemistry package. My work enabled accurate and efficient excited-state and adsorption energy calculations in molecular and periodic systems.

I possess strong verbal, presentation, and written communication skills as demonstrated by extensive **participation in** >17 **conferences** (8 **talks**; 10 **posters**) as well as publishing 10 **scientific articles**.

Prior to joining FSU, I obtained a Master's in Physics from the University of Delhi (India), where I worked with Dr. Debabrata Mishra and published three papers. I obtained my Bachelor's in Physics (Hons) from the University of Delhi as well.

Beyond research, I am deeply involved in **scientific outreach and mentoring**. I create YouTube tutorials and web/Android apps that make complex scientific concepts and computational tools more accessible. I also mentor U.S. high school students in their applications to top US universities. My broader interests include **method and code development for light-matter interactions**, **efficient algorithm design**, and **building intuitive interfaces** for materials modeling and visualization.

Education

Friedrich Schiller University Jena *Jena, Germany*

PhD in Physics (***summa cum laude*** - highest distinction) *June 2019 - March 2024 (4 years 10 months)*

- Thesis topic: "*Density Functional Theory Based Embedding for Molecular and Periodic Systems*" (link)
- Under the supervision of Prof. Dr. Marek Sierka, I developed and implemented efficient methods within the TURBOMOLE program for the study of hybrid systems.
- During my research I became an expert on the implementations and inner workings of quantum chemistry methods like DFT, RT-TDDFT and DFT based embedding techniques coupled with wave function methods.
- Furthermore, I developed a number of practical skills like web app development, graphical designing, video editing, data visualization, data analysis, teaching, automation, etc.
- I also studied deep learning as my supplementary course and designed a very efficient and parallelizable Neural Network library with GPU acceleration.

University of Delhi (Sri Venkateswara College) *New Delhi, India*

Master of Science (MSc) Physics *July 2016 - July 2018 (2 years)*

- Completed a project on density functional theory and material modeling that resulted in two publications in 2019
- Specialized in Nanoscience
- Ranked 3rd in the Physics department of my college

University of Delhi (Acharya Narendra Dev College) *New Delhi, India*

B.Sc (Honours) Physics *July 2013 - July 2016 (3 years)*

- Aggregate percentage: 87.08
- Ranked second in the Physics department of my college (Acharya Narendra Dev College)
- Earned the D.C. Arora meritorious Scholarship, Acharya Narendra Dev College (Apr 2016)
- Was an active member of the Physics society there and held various posts

Work Experience

Indian Institute of Science *Bengaluru, India*

Postdoctoral Researcher *1st August 2024 - present*

- I develop graph neural network-based machine learning interatomic potentials (MLIPs) for investigating thin film deposition and for materials design.
- Developed MLIP Playground, a no-code web application to run atomistic simulations for molecules and materials using state-of-the art machine learning interatomic potentials.
- Perform extensive first-principles (DFT, AIMD and NEB) calculations for reaction pathways and transition state barriers.
- Perform molecular dynamics simulations powered by foundation MLIPs for various properties such as radial distribution functions, density, and so on.
- Served as a teaching assistant for a number of courses:
  - Quantum-Mechanical Modeling of Nanomaterials (CH 253): Conducted tutorials on Quantum ESPRESSO and graded assignments and student exams.
  - AICTE Faculty Development Program (FDP) titled "Application of Machine Learning for Solving Challenging Engineering Problems": Conducted hands-on tutorials on training ML models.
  - Currently serving as a teaching assistant for an NPTEL course on "Machine Learning for Core Engineering Disciplines" where I contribute by creating question papers, assignments, tutorials and reviewing course materials and lectures.

Friedrich Schiller University Jena *Jena, Germany*

Wissenschaftlicher Mitarbeiter (Scientific Employee) *4th June 2019 - 5th April 2024 (4 yrs 10 mos)*

- I developed computationally efficient ab-initio methods and codes to study the properties of hybrid systems. I mainly programmed in Fortran and Python for this role
- Furthermore, I served as a teaching assistant for a number of courses:
  - Modelling and Simulation (Curriculum included basics of quantum mechanics, overview of standard algorithms utilized in quantum chemistry codes such as geometry optimization, and so on.)
  - Basics of Stochastics and Experimental Design
  - Algorithms for Scientific Computing (Curriculum included: Python programming, introduction to machine learning, theory and applications of classical ML models such as SVM, decision trees, and so on.)

  As a teaching assistant, I created exercise sheets and examination papers, conducted weekly tutorials, and graded answer sheets. Additionally, I also deveoped course materials for the course on machine learning and Python.

Phys Whiz (Self-Employed)

Content Creator and Founder *January 2016 - present*

- Founded Phys Whiz to create content like tutorials and lectures on physics, computational material science, and scientific computing
- Currently at ~ 20.4k subscribers on YouTube and ~ 21k followers on Instagram
- Acquired various practical skills through this endeavour like image and video editing, graphic designing, animations, basic social media marketing and management skills
- The YouTube channel has garnered 3.6 Million views (approximately)

BragitOff.com (Self-Employed)

Blogger and Founder *June 2014 - present*

- Owner and author of bragitoff.com, an educational blog, especially for physics students with a focus on computational material science, numerical techniques, and scientific computing
- The blog gets decent traffic with > 30k monthly views
- Searching '*bragitoff.com*' on Google Scholar gives 28 unique results that have cited various blog posts of mine

Awards and Achievements

2026	**Best Oral Presentation,** Awarded for my talk at IISc Chemical Engineering Symposium	*IISc, India*
2019	**Highly Downloaded Paper,** My paper on CrysX was among the top 10 percent of most downloaded papers published in Journal of Applied Crystallography between January 2018 and December 2019	*India*
2025	**Top Viewed Article,** Paper investigating high harmonic generation in molecular thin films was one of the most viewed article among the works published in Advanced Optical Materials between January 1 to December 31 2023	–
2024	**Summa Cum Laude,** Grade awarded for PhD Thesis	*Germany*
2024	**Travel and Accommodation Bursary,** Awarded for presenting my work at Turbomole 2024 Conference	*UK*
2024	**3.6 Million Views and 20.7k Subscribers,** on YouTube channel, where I share my knowledge on computational materials science, physics and scientific computing	*Online*
2022	**Travel Bursary,** Awarded for presenting a talk at ETSF 2022 Conference	*Germany*
2021	**Best Oral Presentation,** Awarded for my talk at EMRS Fall 2021 Meeting	*Germany*
2019	**Highly Downloaded Paper,** My paper on CrysX was among the top 10 percent of most downloaded papers published in Journal of Applied Crystallography between January 2018 and December 2019	*India*
2017	**Rank #3,** Ranked at the 3rd position in the Physics department of my college during M.Sc. Physics	*India*
2016	**DC Arora Scholarship,** Awarded for being a meritorious student during B.Sc. Physics	*India*
2016	**Rank #2,** Ranked at the 2nd position in the Physics department of my college during B.Sc. Physics	*India*

Publications

Here is a link to my Google Scholar (Citations: >362, h-index: 6 at the time of creating the CV)

- *Density Functional Theory for Molecular and Periodic Systems in TURBOMOLE: Theory, Implementation, and Applications*
  M. Sharma, Y. J. Franzke, C. Holzer, F. Pauly, and M. Sierka
  J. Phys. Chem. A (accepted) 129, 39, 9062–9083 (**2025**)

- *Tailored Vapor Deposition Unlocks Large-Grain, Wafer-Scale Epitaxial Growth of 2D Magnetic CrCl3*
  V. Kumar, A. Jangid†, **M. Sharma**†, M. Verma, J. Pasyanthi, K. S. Kumar, P. Sharma, E. O. Chiglintsev, M. I. Panin, S. N. Punnathanam, A. I. Chernov, A. G. Rajan, A. Singh
  Submitted to Adv. Mater., (preprint available on arxiv) (**2025**)

- *Optical Gaps of Ionic Materials from GW/BSE-in-DFT and CC2-in-DFT*
  M. Sharma, and M. Sierka
  J. Chem. Theo. Comput. 20, 21, 9592-9605 (**2024**)

- *TURBOMOLE: Today and Tomorrow*
  Y. J. Franzke, C. Holzer, J. H. Andersen, T. Begušić, F. Bruder, S. Coriani, F. Della Sala, E. Fabiano, D. A. Fedotov, S. Fürst, S. Gillhuber, R. Grotjahn, M. Kaupp, M. Kehry, M. Krstić, F. Mack, S. Majumdar, B. D. Nguyen, S. M. Parker, F. Pauly, A. Pausch, E. Perlt, G. S. Phun, A. Rajabi, D. Rappoport, B. Samal, T. Schrader, **M. Sharma**, E. Tapavicza, R. S. Treß, V. Voora, A. Wodyński, J. M. Yu, B. Zerulla, F. Furche, C. Hättig, M. Sierka, D. P. Tew, and F. Weigend
  J. Chem. Theo. Comput. **19**, 20, 6859-6890 (**2023**) [**HIGHLY CITED**]
  Note: The author list for the above publication was determined using alphabetical order, with the exception of the first two authors and the last five corresponding authors.

- *Resonance Effect in Brunel Harmonic Generation in Thin Film Organic Semiconductors*
  W. Li, A. Saleh, **M. Sharma**, C. Huenecke, M. Sierka, M. Neuhaus, L. Hedewig, B. Bergues, M. Alharbi, H. ALQahtani, A. M. Azeer, S. Graefe, M. F. Kling, A. F. Alharbi, and Z. Wang
  Adv. Optical Mater. 2203070 (**2023**) [**ON COVER and TOP VIEWED ARTICLE**]

- *Efficient Implementation of Density Functional Theory based Embedding for Molecular and Periodic Systems using Gaussian Basis Functions*
  M. Sharma, and M. Sierka
  J. Chem. Theo. Comput. 18, 11, 6892-6904 (**2022**) [**ON SUPPLEMENTARY COVER and ONE OF THE MOST VIEWED ARTICLES IN 30 DAYS OF PUBLICATION**]

- *Real-time time-dependent density functional theory using density fitting and the continuous fast multipole method*
  C. Mueller, **M. Sharma**, and M. Sierka
  J. Comput. Chem. **41**, 2573–2582 (**2020**)

- *CrysX: crystallographic tools for the Android platform*
  M. Sharma, and D. Mishra
  J. Appl. Cryst. **52**, 1449-1454 (**2019**) [**ON COVER, TOP DOWNLOADED ARTICLE**] 🔗
- *First-principles study of the structural and electronic properties of bulk ZnS and small ZnnSn nanoclusters in the framework of the DFT+U method*
  M. Sharma, D. Mishra, and J. Kumar
  Phys. Rev. B **100**, 045151 (**2019**) 🔗
- *DFT+U study of small ZnO nanoclusters*
  M. Sharma, and D. Mishra
  AIP Conf. Proc. **2142**, 110025 (**2019**) 🔗

Review Activities

Served as a peer reviewer for the following journals published by the American Chemical Society:

- *The Journal of Physical Chemistry A*
- *ACS Omega*

Code Development

Contributions

TURBOMOLE	DFT based embedding coupled with WFT and RT-TDDFT methods within the RIPER module of the popular TURBOMOLE package	🔗 www.turbomole.org/

Independently Developed Libraries and Android/PC/Web Applications

PyFock	An efficient density functional theory package based on Gaussian basis functions and supports multi core and GPU acceleration	🔗*GitHub link*
MLIP Playground	A web app to run, test and compare 22 state-of-the-art universal machine learning interatomic potentials (MLIPs) for atomistic simulations of molecules and materials	🔗*Web App link*
CrysX-NN	An efficient neural network library, developed from scratch that supports parallelization and GPUs	🔗*GitHub link*
CrysX-3D Viewer	A molecule and crystal viewer that renders high quality visualizations using complex shaders developed using Unity gaming engine. Avaliable on Android, Windows, Mac and Linux	🔗*Project Home page*
CrysX-AR	An Android app for augmented reality visualization of molecules and crystals	🔗*Google Play Store link*
CrysX-Crystallographic Tools	A set of crystallographic tools (XRD pattern simulation, CIF creator/parser, equation of state fitting, etc.) available as an Android app	🔗*Google Play Store link*
CrysX-Demo DFT based Embedding	Online demo of frozen density embedding and projection based embedding	🔗*Web App link*
RIPER-Tools	An online set of tools that allows to create input files for the RIPER module of TURBOMOLE from MaterialsProject or PubChem database	🔗*Web App link*
VASP-GUI	An online GUI for VASP input preparation and parsing/visualizing output files	🔗*Web App link*
CrysX-CompChem File Converter	Web app that allows inter-conversion between various chemical file formats in current use	🔗*Web App link*
Basis Set Converter	Web app to inter-convert between various basis set formats, powered by Basis Set Exchange	🔗*Web App link*
The Math App	A suite of mathematical tools that has the potential to act as a substitute for Computer softwares like Matlab/Scilab on Android devices	🔗*Google Play Store link*
ML: Microstructure Classification Demo	A web demo app of a neural network (crysx_nn) model trained to classify microstutures	🔗*Web App link*
ML: MNIST_Plus Digit Classification Demo	A web app that classifies user given handwritten digits using a convolutional network model (PyTorch) trained on a modified MNIST dataset	🔗*Web App link*

Conferences, Workshops and Seminars

Talk	IISc Chemical Engineering Symposium (link) 🏆**BEST ORAL PRESENTATION AWARD**	24 Jan 2026
Talk	APS Global Physics Summit 2025 (link)	18 Mar 2025
Attended	IISc-Fujitsu Workshop on Quantum Computing, IISc Bengaluru **India** (link)	23-24 Jan 2025
Attended	AI/ML Workshop 2025, IISc Bengaluru **India** (link)	07-08 Jan 2025
Talk	TURBOMOLE Users Meet Developers Conference, Oxford, **UK** (link)	19 Sep 2024
Lecture+Tutorials	Mastering DFT: A Hands-on Training Workshop, Janardan Singh Foundation (ONLINE)	27 Jul 2024
Poster 🔗	17th International Congress of Quantum Chemistry 2023 in Bratislava, **Slovakia** (link)	25 Jun-01 Jul 2023
Talk	VISTA Seminars 2022 (VIRTUAL (link)	30 Nov 2022
Poster 🔗	BIOVIA Conference 2022 (VIRTUAL (link)	11-13 Oct 2022
Poster 🔗	ICQNN 2022 Conference in Jena, **Germany** (link)	05-09 Sep 2022
Poster 🔗	Psi-K 2022 Conference at EPFL in Lasuanne, **Switzerland** (link)	22-25 Aug 2022
Talk 🔗	25th ETSF Workshop on Electronic Excitations 2022 in Leuven, **Belgium** (link)	13-17 Jun 2022
Talk 🔗	Turbomole Developers Seminar Series 2021-2022	21 Feb 2022
Talk	NOA Spring Meeting 2022 (ONLINE) (link)	21-23 Feb 2022
Talk	Computational Methods in Materials Science (CMMS 2021) (ONLINE) (link)	24-25 Sep 2021
Poster	57th Symposium on Theoretical Chemistry (STC 2021) (ONLINE) (link)	20-24 Sep 2021
Talk 🔗	EMRS Fall 2021 meeting (Online) 🏆**BEST ORAL PRESENTATION AWARD**🏆 (link)	20-23 Sep 2021
Talk 🔗	The Materials and Molecular Modelling Hub++ Annual Conference 2021 (ONLINE) (link)	14-15 Sep 2021
Talk 🔗	DokDok Lite 2021 in Jena, Germany (link)	01-03 Sep 2021
Poster	International Workshop on Recent Developments in Electronic Structure (ES21) (ONLINE) (link)	12-15 Jul 2021
Poster	eSSENCE-eMMC eMeeting MMMM 2021 (Online) (link)	07-08 Jun 2021
Attended	International Workshop on Computer-Aided Materials Discovery (Weekly Online ZOOM Webinars) (link)	27 May-24 Jun 2021
Talk	NOA CRC 1375 Spring Meeting (ONLINE) (link)	15-17 Feb 2021
Attended	Intel® Software Development Tools for HPC (Webinar) (link)	11-20 Nov 2020
Attended	Intel® Software Development Tools for Artificial Intelligence (Webinar) (link)	17 Nov 2020
Attended	NOA Fall PhD School (ONLINE) (link)	26-28 Oct 2020
Poster+Presentation	NOA Spring School and PI Workshop in Jena, **Germany** (link)	02-06 Mar 2020
Attended	NOA seminar by Dr. Heiko Appel (MPI Hamburg) in Jena, **Germany** (link)	21 Jan 2020
Attended	24th ETSF Workshop on Electronic Excitations in Jena, **Germany** (link)	16-20 Sep 2019
Poster	ICABS 2019 in Bhiwani, **India** (link)	07-09 Feb 2019
Poster	6th ISIF 2017 in New Delhi, **India** (link)	13 Dec 2017

Skills

Programming languages	C, C++, C#, Python, FORTRAN, Java, shell scripting
DFT methods development	PySCF, TURBOMOLE
Quantum Chemistry packages	Quantum ESPRESSO, PySCF, TURBOMOLE, NWChem, Serenity, ORCA, VASP
Molecular Dynamics packages	LAMMPS, ASE
Modeling and visualization	VESTA, Avogadro, Jmol, VMD, CrysX-3D Viewer, BURAI, Py3Dmol, ASE
Machine/Deep Learning	scikit-learn, TensorFlow, PyTorch, Nequip, MACE, FairChem UMA, ORB, CrysX-NN
App development	Android, Windows
Web development	Wordpress, HTML
Data processing/wrangling	pandas, numpy
Data visualization	matplotlib, seaborn
Outreach	YouTube videos, Blog posts, Instagram posts
Debugging and profiling	ARM forge for FORTRAN, VS code for python
Miscellaneous	Video editing, Molecular animations,Graphic designing, Photo editing, Git, MS Excel
Documentation	Markdown, LaTeX/Overleaf, Jupyter notebooks, MS Word, MS Powerpoint
Soft Skills	Time Management, Teamwork, Problem-solving, Documentation, Engaging Presentation

Social Media

LinkedIn	https://www.linkedin.com/in/manassharma07
Blog	https://bragitoff.com/
YouTube	https://www.youtube.com/@PhysWhiz
Twitter	https://twitter.com/manassharma07
GitHub	https://github.com/manassharma07/
Instagram	• https://www.instagram.com/phys.whiz • https://www.instagram.com/ducktape07/ • https://www.instagram.com/crysx_3d/
Facebook	• https://www.facebook.com/ducktape07 • https://www.facebook.com/bragitoff/ • https://www.facebook.com/physwhizforum/
Google Scholar	https://scholar.google.com/citations?user=WYOEL94AAAAJ&hl=en
ORCID	https://orcid.org/0000-0002-5346-6280
Researchgate	https://www.researchgate.net/profile/Manas-Sharma-5

Languages

English	Bilingual proficiency
Hindi	Native proficiency
German	Elementary proficiency

References

PhD Supervisor

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Postdoctoral Supervisor

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Master's Supervisor

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References available upon request.