Manas Sharma

PhD (Physics)

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Research Interests

My passion lies in **developing codes and methods** to model the **light-matter interaction of hybrid systems**. More specifically, I am working on improving and accelerating **quantum embedding** techniques for molecular and periodic systems. A core focus of my Ph.D. has been on implementing **density functional theory (DFT) based embedding techniques** and coupling them to real time-time dependent DFT (**RT-TDDFT**) and wavefunction theory (**WFT**) methods. Most notably, I was able to calculate the excitation energies of solvated molecules and adsorption energies of **molecule-periodic** systems using **WFT-in-DFT** method at only a fraction of cost of a traditional calculation. More recently, my work has been focused on accurate molecule-in-periodic embedding and high harmonic generation via RT-TDDFT. Recently, I have also started taking interest in **deep learning** and created a performant neural network library from scratch which supports parallelization and GPUs. I am also experienced in creating GUIs for material modeling, visualizations and input file creations.
Besides all this, I love making YouTube tutorials, web & Android apps, and computer software/libraries for researchers and students.

About me

I am currently seeking postdoctoral positions in the fields of computational material science or computational chemistry. I recently defended my PhD thesis (in Physics) from Friedrich Schiller University Jena (FSU) in Germany, with the highest distinction of *summa cum laude*. I was very fortunate to be supervised by Prof. Dr. Marek Sierka.

During my PhD, I got the opportunity to **participate** in over **17 conferences**, delivering **7 talks** and presenting **10 posters**. This experience helped me in honing my communication skills, both verbal and written. Additionally, I have authored **7 scientific articles** that have been published in reputed peer-reviewed journals.

Prior to joining FSU, I obtained a Master's in Physics from 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.

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. 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.
- Furthermore, I served as a teaching assistant for a number of courses:
  - Modelling and Simulation
  - Basics of Stochastics and Experimental Design
  - Algorithms for Scientific Computing

  As a teaching assistant, I created exercise sheets and examination papers, conducted weekly tutorials, and graded answer sheets.

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

TURBOMOLE *Remote*

Contractual Developer *5th April 2024 - present*

- Implementing gradients for Hartree-Fock exchange for molecular and periodic systems

Friedrich Schiller University Jena *Jena, Germany*

Wissenschaftlicher Mitarbeiter (Scientific Employee) *3rd June 2019 - 4th April 2024 (4 yrs 10 mos)*

- I develop computationally efficient ab-initio methods and codes to study the properties of hybrid systems. I mainly program in Fortran and Python for this role

Phys Whiz (Self-Employed)

Content Creator and Founder *January 2016 - present (6 yrs 10 mos)*

- Founded Phys Whiz to create content like tutorials and lectures on physics, computational material science, and scientific computing
- Currently at ~ 18k subscribers on YouTube and ~ 22k 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 3.2 Million views (approximately)

BragitOff.com (Self-Employed)

Blogger and Founder *June 2014 - present (8 yrs 5 mos)*

- 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

Publications

Here is a link to my Google Scholar

- *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**)
  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**)

- *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**]

- *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 PAGE**]

- *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 Conference Proceedings 2142, 110025 (**2019**)

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

CrysX-NN	An efficient neural network library 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 tools that allows to create input files for the RIPER module of TURBOMOLE from MaterialsProject or PubChem database	🔗*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

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
Modeling and visualization	VESTA, Avogadro, Jmol, VMD, CrysX-3D Viewer, BURAI, Py3Dmol
Machine/Deep Learning	scikit-learn, TensorFlow, PyTorch, 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 available upon request.