



# Manas Sharma

PHD CANDIDATE

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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 a fifth-year PhD student in Physics at Friedrich Schiller University Jena (FSU) Germany, fortunate to be advised by Prof. Marek Sierka.

I possess strong verbal, presentation, and written communication skills as demonstrated by extensive **participation in >17 conferences (7 talks; 10 posters)** as well as publishing **7 scientific articles**.

Prior to joining FSU, I obtained a Master's in Physics from University of Delhi (India), where I worked with Dr. Debabrata Mishra. I published two papers with him.

I obtained my Bachelor's in Physics (Hons) from the University of Delhi as well. I am originally from a small, but beautiful town Haldwani, a few minutes from Nainital in India.

## Education

### Friedrich Schiller University Jena

Jena, Germany

PhD Candidate in Physics

June 2019 - present (3 years 4 months)

- Under the supervision of Prof. Marek Sierka, I develop and implement 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

### Friedrich Schiller University Jena

Jena, Germany

Wissenschaftlicher Mitarbeiter (Scientific Employee)

June 2019 - present (3 yrs 4 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 ~ 17k subscribers on YouTube and ~ 24k 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 2.9 Million views (approximately)

### BragitOff.com (Self-Employed)

Blogger and Founder

June 2014 - present (8 yrs 5 mos)

- Owner and author of [bragitoff.com](http://bragitoff.com), an educational blog, especially for physics students with a focus on computational science and scientific computing
- The blog gets decent traffic with around 50k monthly views (35k unique visitors).
- Last year (2021) the blog received 600k views

## 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. Furst, 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.* xxxx (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 ZnSn 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/](http://www.turbomole.org/)

### Independently Developed Libraries and Android/PC/Web Applications

<b>CrysX-NN</b>	An efficient neural network library from scratch that supports parallelization and GPUs	<a href="#">🔗GitHub link</a>
<b>CrysX-3D Viewer</b>	A molecule and crystal viewer that renders high quality visualizations using complex shaders developed using Unity gaming engine. Available on Android, Windows, Mac and Linux	<a href="#">🔗Project Home page</a>
<b>CrysX-AR</b>	An Android app for augmented reality visualization of molecules and crystals	<a href="#">🔗Google Play Store link</a>
<b>CrysX-Crystallographic Tools</b>	A set of crystallographic tools (XRD pattern simulation, CIF creator/parser, equation of state fitting, etc.) available as an Android app	<a href="#">🔗Google Play Store link</a>
<b>CrysX-Demo DFT based Embedding</b>	Online demo of frozen density embedding and projection based embedding	<a href="#">🔗Web App link</a>

## Other Tools and Projects

<b>CrysX-CompChem File Converter</b>	Web app that allows inter-conversion between various chemical file formats in current use	<a href="#">🔗Web App link</a>
<b>Basis Set Converter</b>	Web app to inter-convert between various basis set formats, powered by Basis Set Exchange	<a href="#">🔗Web App link</a>
<b>The Math App</b>	A suite of mathematical tools that has the potential to act as a substitute for Computer softwares like Matlab/Scilab on Android devices	<a href="#">🔗Google Play Store link</a>
<b>ML: Microstructure Classification Demo</b>	A web demo app of a neural network (crysx_nn) model trained to classify microstructures	<a href="#">🔗Web App link</a>
<b>ML: MNIST_Plus Digit Classification Demo</b>	A web app that classifies user given handwritten digits using a convolutional network model (PyTorch) trained on a modified MNIST dataset	<a href="#">🔗Web App link</a>

## Conferences, Workshops and Seminars

<b>Poster</b> 🔗	17th International Congress of Quantum Chemistry 2023 in Bratislava, Slovakia ( <a href="#">link</a> )	25 Jun-01 Jul 2023
<b>Talk</b>	VISTA Seminars 2022 (VIRTUAL) ( <a href="#">link</a> )	30 Nov 2022
<b>Poster</b> 🔗	BIOVIA Conference 2022 (VIRTUAL) ( <a href="#">link</a> )	11-13 Oct 2022
<b>Poster</b> 🔗	ICQNN 2022 Conference in Jena, Germany ( <a href="#">link</a> )	05-09 Sep 2022
<b>Poster</b> 🔗	Psi-K 2022 Conference at EPFL in Lausanne, Switzerland ( <a href="#">link</a> )	22-25 Aug 2022
<b>Talk</b> 🔗	25th ETSF Workshop on Electronic Excitations 2022 in Leuven, Belgium ( <a href="#">link</a> )	13-17 Jun 2022
<b>Talk</b> 🔗	Turbomole Developers Seminar Series 2021-2022	21 Feb 2022
<b>Talk</b>	NOA Spring Meeting 2022 (ONLINE) ( <a href="#">link</a> )	21-23 Feb 2022
<b>Talk</b>	Computational Methods in Materials Science (CMMS 2021) (ONLINE) ( <a href="#">link</a> )	24-25 Sep 2021
<b>Poster</b>	57th Symposium on Theoretical Chemistry (STC 2021) (ONLINE) ( <a href="#">link</a> )	20-24 Sep 2021
<b>Talk</b> 🔗	EMRS Fall 2021 meeting (Online) 🏆 <b>BEST ORAL PRESENTATION AWARD</b> 🏆 ( <a href="#">link</a> )	20-23 Sep 2021
<b>Talk</b> 🔗	The Materials and Molecular Modelling Hub++ Annual Conference 2021 (ONLINE) ( <a href="#">link</a> )	14-15 Sep 2021
<b>Talk</b> 🔗	DokDok Lite 2021 in Jena, Germany ( <a href="#">link</a> )	01-03 Sep 2021
<b>Poster</b>	International Workshop on Recent Developments in Electronic Structure (ES21) (ONLINE) ( <a href="#">link</a> )	12-15 Jul 2021
<b>Poster</b>	eSSSENCE-eMMC eMeeting MMMM 2021 (Online) ( <a href="#">link</a> )	07-08 Jun 2021
<b>Attended</b>	International Workshop on Computer-Aided Materials Discovery (Weekly Online ZOOM Webinars) ( <a href="#">link</a> )	27 May-24 Jun 2021
<b>Talk</b>	NOA CRC 1375 Spring Meeting (ONLINE) ( <a href="#">link</a> )	15-17 Feb 2021
<b>Attended</b>	Intel® Software Development Tools for HPC (Webinar) ( <a href="#">link</a> )	11-20 Nov 2020
<b>Attended</b>	Intel® Software Development Tools for Artificial Intelligence (Webinar) ( <a href="#">link</a> )	17 Nov 2020
<b>Attended</b>	NOA Fall PhD School (ONLINE) ( <a href="#">link</a> )	26-28 Oct 2020
<b>Poster+Presentation</b>	NOA Spring School and PI Workshop in Jena, Germany ( <a href="#">link</a> )	02-06 Mar 2020
<b>Attended</b>	NOA seminar by Dr. Heiko Appel (MPI Hamburg) in Jena, Germany ( <a href="#">link</a> )	21 Jan 2020
<b>Attended</b>	24th ETSF Workshop on Electronic Excitations in Jena, Germany ( <a href="#">link</a> )	16-20 Sep 2019
<b>Poster</b>	ICABS 2019 in Bhiwani, India ( <a href="#">link</a> )	07-09 Feb 2019
<b>Poster</b>	6th ISIF 2017 in New Delhi, India ( <a href="#">link</a> )	13 Dec 2017

## Skills

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

## Social Media

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**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/\\_\\_\\_\\_physwhiz\\_\\_\\_\\_](https://www.instagram.com/____physwhiz____)
- <https://www.instagram.com/ducktape07/>
- [https://www.instagram.com/crysx\\_3d/](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

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**English** Bilingual proficiency

**Hindi** Native proficiency

**German** Elementary proficiency

**References available upon request.**