



ADITI SINGH

Contact

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Personal details

Date of Birth - 02/02/1997

Core Qualifications

Programming - Python
Softwares - PySCF, Psi4,
KSPies, n2v, Molpro
Quantum Physicist
Language - English

Education

Banaras Hindu University
Banaras
Master of Science: Physics
2020
Thesis- Photothermal therapy
for Cancer treatment using
MoTe₂
Dissertation in BioPhysics

Experience :

Ph.D.

Nicolaus Copernicus University, Toruń , Poland |Toruń , Poland | Dec 2021 - Current

- Under the supervision of **Ireneusz Grabowski, Eduardo Fabiano(CNR-IMM Lecce), and Szymon Śmiga.**
- I work as a methodological development scientist in density functional theory.
- My goal is to develop a new exchange correlational functional that could be used to obtain chemical accuracy.
- We have developed a new tool that analyses the existing functional and makes us understand how they could be improved, from the insights we focus on developing our new functionals.

Publications :

- Published paper: Aditi Singh and Vignesh Balaji Kumar and Ireneusz Grabowski and Szymon Śmiga, Physically meaningful solutions of optimized effective potential equations in a finite basis set within KS-DFT framework, Book- Polish Quantum Chemistry from Kołos to Now, Chapter 9, Volume 87, 2023, Pages 297-317, Advances in Quantum Chemistry, DOI-<https://doi.org/10.1016/bs.aiq.2023.01.003>
- Understanding the core limitations of second-order correlation-based functionals through: functional, orbital, and eigenvalue-driven analysis, **Journal of Chemical Theory and Computation**, DOI-10.1021/acs.jctc.4c01376
- Submitted: Simplified, Physically Motivated, and Universally Applicable Range-Separation Tuning, **The Journal of Physical Chemistry Letters**.

Accomplishments :

- Best Poster Prize in Twenty-sixth International Workshop on QSCP-XXVI poster entitled: "Estimating the performance of Double Hybrid Functionals with various input densities".

Internships :

- Internship - Italian Institute of technology Center for Biomolecular Nanotechnologies Lecce, Italy Dr. Eduardo Fabiano, 1.09.2023 to 17.09.2023
- Internship – KTH Royal Institute of Technology, Stockholm, Sweden, Prof. Patrick Norman. 1.02.2025 to 28.02.2025

