ANNUAL REPORT – 1st year of education (2023/2024)

Start of education**: *October 1st, 2023***

Doctoral School of Exact and Natural Sciences, NCU in Toruń

"Academia Scientiarum Thoruniensis"

1. Student information

First and last name	Ram Dhari Pandey
Scientific field	Novel pCCD based methods for designing efficient OPV materials
Transcript number	503552
Date of acceptance to doctoral school	1/10/2023

2. Supervisor 1 information

First and last name	Pawel Tecmer
Title/degree	Dr.hab.
Department	Institute of Physics, Faculty of Physics, Astronomy and Informatics

3. Supervisor 2 information

First and last name	
Title/degree	
Faculty/department	

4. Co-supervisor information

First and last name	
Title/degree	
Faculty/department	

5. Information about implementation of teaching program

	course name	no. hours	ECTS	pass/ grade
Module I – basic courses	1. Supervisor mentoring [7404-MP-FIZ]	30	2	ZAL
Module I – Lecture in additional discipline	4. Fundamentals of climate and climate change [7404-SD-NoZIS-FCLIM]	30	3	Passed 4.5
Moduł II – courses improving professional skills	2. Techniques for presenting results and popularizing scientific knowledge	10	1	In progress
	5. Interdisciplinary seminar [7404-KIN]	30	3	In progress
	3. Occupational Safety Health and Ergonomics [9001-eBHP]	8	NA	ZAL Passed
	4. Scientific writing and publishing [7404-FIZ-PPTN]	15	2	Passed 3
	5. Creative thinking [7404-CT]	10	1	ZAL Passed
	6. Occupied Safety Health and Ergonomics [9001-BHP-5SD]	5	NA	ZAL Passed

	7. Organization and financing of research [7404-OFB]	15	2	In progress
Module III – specialistic courses	13. An introduction to computational spectroscopy [0800-COMSPEC1]	30+15	3	Lecture(Passed) 5 Lab(passed) 4.5
	14. Introduction to density functional theory [0800-INDEFUT]	30	3	Passed 5
	15. Introduction to python for Doctoral students [7404-ITP]	30	3	Passed 4.5

6. Information about internships (co-conducting classes)

course: NA	number of hours:

7. Information about internships (conducting classes)

course: NA	number of hours:

8. Publication of a scientific article in a scientific journal, monograph or chapter in monograph/review

I am currently working on the paper titled "Novel pCCD-based approaches for Designing Organic Photovoltaic (OPV) Materials: Electronic Structure and Properties of BN-embedded Polycyclic Aromatic Hydrocarbons (PAHs)." In this work, I have computed ionization potentials (IPs), electron affinities (EAs), and excitation energies for 23 isomers of BN-doped naphthalene using a variety of computational methods. These methods include HF, MP2, CCSD, CCSD(T), IP-EOM-fpCCD, IP-EOM-fpCCSD, EOM-pCCD-CCS, EOM-pCCD+S, EOM-pCCD-LCCD, and EOM-pCCD-LCCSD. These diverse arrays of computational strategies provide a comprehensive understanding of the electronic structure and properties of the BN-embedded PAHs.

Our study focuses specifically on analyzing the impact of BN doping on the ionization potential, electronic affinity, and low-lying singlet and triplet excitations of all twenty-three BN-naphthalene isomers. The calculation results demonstrate consistent and reliable outcomes among the fpCCD, fpCCSD, and CCSD(T) methods, which closely align with experimental values. Furthermore, this study emphasizes the significance of heteroatoms (boron and nitrogen) as a donor and acceptor in shaping optical and electronic properties. This fundamental knowledge is crucial for precisely customizing and designing efficient OPV materials with tailored properties.

9. Active participation (oral presentation or poster) in an international conference, documented in conference materials

Poster presentation:

In September, I will present a poster at the 9th Current Trends in Theoretical Chemistry(CTTC9) conference in Krakow, Poland (1-5 September), followed by another poster presentation at the 19th Central European Symposium on Theoretical Chemistry(CESTC) conference in Sveti Martin Muri, Croatia (11-14 September).

10. Participation in workshops or summer schools

I have participated in a workshop titled "Best Practices in Software Development," which was jointly organized by The Molecular Sciences Software Institute (MOISSI) and Dr. hab. Piotr Żuchowski from the Institute of Physics at Nicolaus Copernicus University. This workshop was specifically intended for doctoral students. The event took place at Hotel UMK, located in Torun, Poland, over a period of four days in February.

11. Co-organization of workshops and scientific conferences

N/A

12. Documented participation of doctoral student in internships or courses that improve qualifications

N/A

13. Financing scientific research of doctoral student from own grants or grants obtained by supervisor/other sources

N/A

14. List of applications sumbitted by doctoral student in university or external contests for funding of trips abroad and/or scientific research

N/A

15. Internships of doctoral student in other scientific centers (including foreign ones, if justified by discipline of student)

N/A

16. Scientific achievements of doctoral student (scientific articles, monographs), which were created in international cooperation

N/A

17. Publishing scientific articles in magazines from first quartile (Q1) or most prestigious publications (for 200 points)

N/A

18. Joint co-supervision of doctoral thesis together with foreign partners

N/A

19. Other activities of doctoral student (e.g. disseminating activities, passive participation in conferences, etc.)

N/A

20. Student's comments on the course of last year of education

An introduction to computational spectroscopy: This course facilitates a deep understanding of Hartree-Fock (HF) theory, Born-Oppenheimer approximation, Koopmans theorem, and Brillouin's theorem. It enhances skills and knowledge of Molpro and Turbomole software, enabling the application of theoretical methods to interpret and predict data effectively.

Scientific Presentation: Improves presentation skills and techniques, crucial for effectively conveying complex scientific concepts to diverse audiences.

Scientific Writing and Publishing: Develops clear, concise writing skills and understanding of the publishing process, essential for effectively communicating research findings.

Python for doctoral students: Enhances computational and coding skills.

Interdisciplinary Seminar: Encourages collaboration and broadens knowledge across various fields, fostering innovative approaches and interdisciplinary research skills.

Fundamentals of Climate and Climate Change: Provides a comprehensive understanding of climate systems and the impacts of climate change.

Creative Thinking: Enhances problem-solving skills and encourages innovative approaches.

Fundamentals of Density Functional Theory: Ensures a robust understanding of basic DFT principles, including the Hohenberg-Kohn theorems and Kohn-Sham equations. it covers various exchange-correlation functionals essential for accurately describing electron interactions within systems.

21. Approval of the report by supervisor/supervisors

(filled out by supervisor/supervisors)

I approve the report of the student.

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signature of supervisor/supervisors

22. Recommendations and comments by School Director

(filled out by School Director)

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signature of School Director

developed by: Renata Drozdowska