# Directorate of Research

# UTTARAKHAND OPEN UNIVERSITY, HALDWANI, 263139

## Ph.D. Progress Report (September 2022 to February 2023)

**Name of the Research Scholar:** Shradha lakhera

**Enrolment No.:** 21240578

**Department:** Department of Physics

**Subject:** Physics

**Date of Registration:** 1st March 2021

**Date of RAC:** 16th August 2022

**Date of RDC:** 28th February 2023

**Title of the Research Work:** Study of Optical and Druglike Properties of Some Organic Molecules

**Name of the supervisor:** Dr. Kamal Devlal

**Duration of the progress report:** September 2022 to February 2023

**Received any fellowship/ scholarship:** No

**Highlight the progress of work during the period of the progress report**

1. Literature survey and planning the method of the experimental work.
2. Identification of the potential compounds for experimental work i.e., 4-aminobenzoic acid, 7-diethylamino 4-methyl coumarin.
3. Performed computational analysis for chemical reactivity and charge transport activity for the selected compounds using density functional theory.
4. Performed experimental demonstrations for NLO activity and photosensitizing ability of the selected molecules.
5. Published and communicated research articles in some highly reputed peer-reviewed journals.
6. Presented research articles at national and international conferences.
7. Received two state-level awards for research.

**Detailed Research work**

1. Computational investigations of optical characteristics of 4-aminobenzoic acid, and 7-diethylamino 4-methyl coumarin were performed and communicated.

2. Computational investigations of non-linear optical characteristics of organic-inorganic hybrid systems developed with the adsorption of gold and silver trimers over the surface if Pentacene-2,5-dione and 2,9-dimethyl quinacridone has been performed and communicated.

3. Experimental work for the spectroscopic techniques of 4-aminobenzoic acid had been carried out in the laboratory of Jaypee institute of information and technology (JIIT), Noida, and Gurukula kangri university, Haridwar.

4. The samples of 4-aminobenzoic acid, and 7-diethylamino 4-methyl coumarin were sent to Dr. T. C. Sabari Girisun, Assistant Professor, Department of Physics, Bharathidasan University, Tiruchirappalli, Tamil Nadu, for the Z-scan experiments in collaboration.

**Published and communicated research articles**

1. S. Lakhera, M. Rana, K. Devlal (2022) Theoretical study on spectral and optical properties of essential amino acids: a comparative study, Opt Quantum Electron. 54:714 https://doi.org/10.1007/s11082-022-04118-4
2. S. Lakhera, M. Rana, K. Devlal, Investigation of Nonlinear Optical Response of Organic Compound Pyrrolidine-2,5-dione, DAE Solid State Physics Symposium. 55 (2022) 585-586
3. S. Lakhera, M. Rana, K. Devlal, Modelling the reactivity of Entrectinib and evaluation of its potential anticancer activity using Molecular Docking approach, DAE Solid State Physics Symposium 55 (2022) 583-584.
4. S. Lakhera, M. Rana, K. Devlal, Influence of Adsorption of Gold and Silver Nanoclusters on Structural, Electronic, and Nonlinear optical properties of Pentacene-5, 12-dione: A DFT study, Opt Quant Electron 55, 178 (2023). https://doi.org/10.1007/s11082-022-04422-z
5. S Lakhera, M Rana, K Devlal, Investigation of the Electrical and Optical Activity of Halogen-substituted 2-nitrotoulene by Density Functional Theory (2022). https://doi.org/10.21203/rs.3.rs-2111123/v1
6. S. Lakhera, K. Devlal, M. Rana, V. Dhuliya, Computational study of non-linear optical and electrical properties of 1,3-dinitropyrene. Opt Quant Electron 55, 85 (2023). https://doi.org/10.1007/s11082-022-04371-7
7. S. Lakhera, M. Rana, K. Devlal, N. Kanagathara, J. Janczak, DFT-Based Solvent Analysis of Organic Heterocyclic 2,9-Dimethyl Quinacridone for Photovoltaic Applications. http://dx.doi.org/10.2139/ssrn.4329946
8. S. Lakhera, M. Rana, K. Devlal, A. Ghosh, In-Silico Investigation of Inhibiting Property of Phytoconstituents of Medicinal Herb 'Aconitum Heterophyllum' Against Omicron Variant of SARSCoV-2, Indian Journal of Traditional Knowledge. https://doi.org/10.21203/rs.3.rs-1637533/v1
9. S. Lakhera, M. Rana, K. Devlal, Investigation of Nonlinear Optical Responses of Organic Derivative of Imidazole: Imidazole-2-carboxaldehyde. International Journal of materials research (Under review).
10. S. Lakhera, K. Devlal, M. Rana, V. Dhuliya, N. Pandey, Behavior of 2,9-Dimethylquinacridone with Adsorbed Gold and Silver Nanoclusters in Different Solvents. Optik (Under review).

**National and international conferences**

1. Presented research work at 17th Uttarakhand state science and technology congress (USSTC) in UCOST, Vigyan Dham, Dehradun in February 2023.
2. Presented research work in 5th Plant science research meet 2022 held at Uttarakhand Open University, Haldwani.
3. Submitted research abstract in IFPAM-2023 1st International Conference on Innovations & Future Prospects of Advanced Materials, conducted by K R Mangalam University, Gurugram.

**Workshops and seminars**

1. Attended workshop and hands-on training on synthesis and characterization of nanocomposites and User acquaintance program by Inter-university acceleratorcenter, New Delhi conducted on 17th October 2022 at Gurukula kangri University, Haridwar.

2. Attended the Hands-on training on Spectroscopic techniques and material structures organized by USERC, held from 29th August to 3rd September 2022.

3. Attended INUP-121 Hands-on training on Synthesis and characterization of solar cell, conducted at IIT Delhi, from 5th to 10th December 2022.

4. Attended INUP-121 5th User awareness workshop on fabrication and characterization of Nanotechnology in online mode, conducted at IIT Delhi, from 6th to 7thJanuary 2023.

**Awards and Honours**

1. Received USERC "Young women scientist excellence award 2022" at the Women scientist conclave 2022-23 held at Dehradun.

2. Short-term project approved at National research facility (NRF) at IIT Delhi under Indian nanoelectronics user program for the synthesis of Dye-synthesized solar cell using 7-diethylamino 4-methyl coumarin.

Shradha

Date: 28.2.23

Signature and Name of Scholar

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Signature and Name of Supervisor

# Ph.D. Progress Report (March 2023-August 2023)

## Directorate of Research

## UTTARAKHAND OPEN UNIVERSITY, HALDWANI, 263139

1. **Name of the Research Scholar:** Shradha Lakhera
2. **Enrolment No.:** 21240578
3. **Department:** Department of Physics, School of Sciences, Uttarakhand Open University
4. **Subject:** Physics
5. **Date of Registration:** 1st March 2021
6. **Date of RDC:** 18th August 2023
7. **Title of the Research Work:** Study of organic materials for Nonlinear optical and laser limiting applications
8. **Name of the supervisor:** Dr. Kamal Devlal
9. **Highlight the progress of work during the period of the progress report**
    - Computational study of nonlinear optical properties of *para*-aminobenzoic acid.
    - Experimental study of nonlinear optical and laser limiting study of para-aminobenzoic acid
    - Computational study of the nonlinear optical behavior of 7-diethylamino 4-methyl coumarin.
    - Presented research papers at one national and one international conference.
    - Published 7 full-length research articles in peer-reviewed journals related to the research work.

**Future Plans**

1. Experimental study for nonlinear optical properties and optical limiting behavior of 7-diethylamino 4-methyl coumarin.
2. Computational study for nonlinear optical properties and optical limiting behavior of volumetric ratio solutions of para-aminobenzoic acid and 7-diethylamino 4-methyl coumarin.
3. Experimental study for nonlinear optical properties and optical limiting behavior of volumetric ratio solutions of *para*-aminobenzoic acid and 7-diethylamino 4-methyl coumarin

**Published and submitted articles**


1. S. Lakhera, M. Rana, K. Devlal, S. Sharma, P. Chowdhury, V. Dhuliya, S. Panwar, Sagar L. P. Purohit, A. Dhanusha, T. C. Girisun, Exploring the Nonlinear Optical Limiting Activity of Para-Aminobenzoic Acid by Experimental and DFT Approach. Journal of Photochemistry and Photobiology A: Chemistry. (2023) 114987. https://doi.org/10.1016/j.jphotochem.2023.114987

2. S. Lakhera, M. Rana, K. Devlal, Influence of Adsorption of Gold and Silver Nanoclusters on Structural, Electronic, and Nonlinear optical properties of Pentacene-5, 12-dione: A DFT study, Opt Quant Electron 55 (2023) 178. https://doi.org/10.1007/s11082-022-04422-z

3. S. Lakhera, M. Rana, K. Devlal, Investigation of Nonlinear Optical Responses of Organic Derivative of Imidazole: Imidazole-2-carboxaldehyde, IJMR. (2023). https://doi.org/10.1515/ijmr-2021-8649

4. S. Lakhera, K. Devlal, M. Rana, Investigation of the electronic and optical activity of halogen-substituted 2-nitrotoulene by density functional theory. Opt Quant Electron 55 (2023) 292 (2023). https://doi.org/10.1007/s11082-023-04569-3

5. S. Lakhera, K. Devlal, M. Rana, V. Dhuliya, Computational study of non-linear optical and electrical properties of 1,3-dinitropyrene. Opt Quant Electron 55 (2023) 85 (2023). https://doi.org/10.1007/s11082-022-04371-7

6. S. Lakhera, M. Rana, K. Devlal, N. Kanagathara, J. Janczak, Photovoltaic Characteristics of Organic Heterocyclic2,9-dimethyl Quinacridone in Different Solvents Using DFT Approach, Journal of Photochemistry and Photobiology A: Chemistry. (2023) 114664. https://doi.org/10.1016/j.jphotochem.2023.114664

7. S. Lakhera, K. Devlal, M. Rana, V. Dhuliya, N. Pandey, Non-Linear Optical Behavior of 2,9-Dimethylquinacridone with Adsorbed Gold and Silver Nanoclusters, Optik. (2023) 170983. https://doi.org/10.1016/j.ijleo.2023.170983




Devlal

**Conferences and seminars**

1. Research work was presented in a poster presentation at the Indian Science Congress Association: Haridwar Chapter, hosted by Gurukula Kangri (Deemed to be university), Haridwar, Uttarakhand on 19th March 2023.

2. Presented poster in IFPAM-2023, 1st International Conference on Innovations & Future Prospects of Advanced Materials, conducted by K R Mangalam University, Gurugram on 23rd March 2023.

Shradha

SHRADHA LAKHERA

Signature and Name of Scholar

Date: 18/Aug/2023

(Kamal Dodal)

Signature and Name of Supervisor

## Directorate of Research

## UTTARAKHAND OPEN UNIVERSITY, HALDWANI, 263139

## PhD Progress Report

**Name of the Research Scholar:** Shradha lakhera

**Enrolment No.:** 21240578

**Department:** Department of Physics

**Subject:** Physics

**Date of Registration:** 1st March 2021

**Date of RAC:** 16th August 2022

**Title of the Research Work:** Study of Optical and Biological Properties of Some Organic Molecules and Their Applications

**Name of the supervisor:** Dr. Kamal Devlal

**Duration of the progress report:** September 2021 to August 2022

**Received any fellowship/ scholarship:** No

**Highlight the progress of work during the period of progress report**

1. Identification of the research topic i.e., Study of Optical and Biological Properties of Some Organic Molecules and Their Applications
2. Literature survey and current progress in this field.
3. Identification of the availability of online softwares for computational methods.
4. Identification of the theoretical (computational) study and experimental techniques.
5. Application of software for some trial organic materials.
6. Published and communicated research articles on some highly reputed peer reviewed journals.
7. Presented research articles in three conferences.
8. Developed national and international collaborations.

Date: 16/08/2022

Shradha

Shradha Lakhera
Signature and Name of Scholar

16.8.22 (Dr Kamal Devlal)
Signature and Name of Supervisor

Professor P. D. Pant
(Chairman)

Dr Gauri Negi
(Member)

Dr Meenakshi Rana
(Invited member)

Signature
Director, School of Sciences