The report should be sent (in the sealed envelope) to the Exam Controller, Uttarakhand Open University, Teen pani Bypass Road, Haldwani (Nainital) -263139.

UOU/Research/Physics /2024/01   **DATE: 17/05/2024**

PROFORMA FOR THE WRITING Ph. D. THESIS REPORT

1- Name of the Candidate **Shradha Lakhera** Registration No. 21240578".
2- Subject: **Physics**
3- Name of the Doctorate Degree: Ph. D.
4- Title of thesis : **"Implementation of Financial Technologies in Public Sector Bank and its Adoption amongst Customers: A Descriptive Study"**
5- Name of the examiner with full postal address **Prof. P.S. Bisht, Dept. of Physics, SSJ University, Almora, Pin- 263601 Uttarakhand.**

Note – Under the ordinance relating to Doctorate Degree a thesis shall comply with the following conditions and the examiners are requested that in case they approve of a thesis for the degree, is should be definitely mentioned in the report that the thesis complies with these requirements.

(a) It must be a piece of research work characterized either by the discovery of facts or by a fresh approach towards the interpretation of facts or theories. In either case it should evince the candidate's capacity for critical examination and sound judgment.

(b) It shall be satisfactory in point of language and presentation of subject matter. The examiners will also indicate whether the thesis is suitable for publication in its present form with or without amendments.

IMPORTANT

The Examiner is requested to recommend definitely weather.

(a) The candidate is admitted to the degree.
                                    Or
(b) The candidate should improve and resubmit the thesis.
                                    Or
(c) The thesis should be rejected.

REPORT

Dated 6/6/2024

(Signature of the Examiner)

(If necessary blank sheets may be added to complete the report)

Report

The present thesis entitled **"Computational and experimental studies of some functional group rich organic nonlinear optical materials and their applications"** submitted by **Shradha Lakhera** for the award of **Doctor of Philosophy** in Physics to **Uttarakhand Open University, Haldwani** contains five chapters.

First chapter is an introductory which contains basic information of the subject and the literature sited in the present thesis. The research problem is well defined and the objectives of research stated clearly.

In chapter 2, author have mentioned the review of literature in the thesis and relevant to the identified problem. It is clearly established in the current knowledge.

In chapter 3 contains the materials and methods used in the present work. The organic nonlinear optical materials selected for the present research work is clearly mentioned and the computational and experiments used in the present study are well defined. The details of density functional theory are also well defined to generate critical new information. The techniques used in present research work is a computer added and density functional theory including different experiments techniques like UV visible spectroscopy, solar simulator, optical limiting and fill factor etc. are appropriate.

In chapter 4, author has briefly written the conclusion and Future Scopes of the present work. The conclusion and future scopes and summary of the thesis have been summarised properly and the conclusion drawn are appropriate.

The author has already published papers in the International Journal of repute based on the present work. The candidate presented her work very systematically and the literacy presentation of the thesis is good. **Hence, the thesis submitted by Shradha Lakhera fulfilment of the requirements for the award of Doctor of Philosophy degree in Physics is in my opinion quite satisfactory and should be accepted for the award of Ph. D. degree.**

Date: - 06/06/2024

Place: - ALMORA

Prof. (Dr.) P. S. Bisht

The report should be sent (in the sealed envelope) to the Exam Controller, Uttarakhand Open University, Teen pani Bypass Road, Haldwani (Nainital) -263139.

UOU/Research/Physics /2024/01   DATE: 17/05/2024

PROFORMA FOR THE WRITING Ph. D. THESIS REPORT

1- Name of the Candidate **Shradha Lakhera** Registration No. 21240578".
2- Subject: **Physics**
3- Name of the Doctorate Degree: Ph. D.
4- Title of thesis : **Computational and experimental studies of some functional group rich organic nonlinear optical materials and their applications.**
5- Name of the examiner with full postal address **Prof. L.P. Purohit, Dept. of Physics, Gurukula Kangri Vishwavidyalaya, Haridwar 249404**

Note – Under the ordinance relating to Doctorate Degree a thesis shall comply with the following conditions and the examiners are requested that in case they approve of a thesis for the degree, is should be definitely mentioned in the report that the thesis complies with these requirements.

(a) It must be a piece of research work characterized either by the discovery of facts or by a fresh approach towards the interpretation of facts or theories. In either case it should evince the candidate's capacity for critical examination and sound judgment.

(b) It shall be satisfactory in point of language and presentation of subject matter. The examiners will also indicate whether the thesis is suitable for publication in its present form with or without amendments.

IMPORTANT

The Examiner is requested to recommend definitely weather.

✓(a) The candidate is admitted to the degree.
                    Or
(b) The candidate should improve and resubmit the thesis. ✗
                    Or
(c) The thesis should be rejected. ✗

REPORT

Dated ..04. 06. 2024...... *Report attached .*

....
(Signature of the Examiner)

(If necessary blank sheets may be added to complete the report)

PROF. L.P. PUROHIT
Department of Physics
Gurukula Kangri Vishwavidyalaya
Haridwar-249404(U.K.)

Thesis title: Computational and experimental studies of some functional group rich organic nonlinear optical materials and their applications.

Name of the candidate: **Shradha Lakhera**
Degree program: **PhD**
Enrolment no: **21240578**
Year: **2024**

The research work reported in this thesis comprises selection of the potential functional group-rich organic compounds, computational and experimental study of the selected compounds such as NLO, OL, PV, and CADD.

The PV parameters like LHE, FF, Voc, EQE are introduced in the Chapter 1. Along with these, the CADD techniques like molecular docking and MD simulation are defined.

Chapter 2 reports the literature and the software and databases like Gaussian, AutoDock, PubChem, etc., used for the computational studies. The spectroscopic tools, like absorption spectroscopy, vibrational spectroscopy, and Z-Scan spectroscopy were used in this research work.

The computational analysis in Chapter 3 was done using DFT calculations for all the selected organic compounds like fatty alcohols, amino acids, aminobenzoic acids, coumarin derivatives, plant phytochemicals, pyrene and toluene derivatives and the computational techniques have been applied to account the theoretical values of polarizability parameters.

Different spectroscopic tools were then employed for the experimental demonstration of the NLO and OL applications. The experimental calculations involve the absorption, vibrational, and Z-Scan spectroscopy analysis. The results from the experimental demonstration of these techniques have been reported in Chapter 4.

The PV application of the selected compound selected was further used as a photosensitizing material in DSSC. DSSCs of different concentrations of sensitizing material were fabricated and tested. Characterizations like solar simulation under 1 Sun illumination, EQE, and absorption spectroscopy were experimentally performed for validating the working of the fabricated devices. The compound selected for NLO properties are further investigated for the property of CADD.

The pharmacokinetic properties were analyzed for the initial screening of druglikeness of the compound. Molecular docking was performed for checking the inhibitory potentiality of the clitorin against the AD macromolecules. The docking parameters such that binding affinity, hydrogen and hydrophobic bonds, inhibition constant, drieding energy, etc., accounted the binding of the drug candidate at the binding sites of the macromolecule. The stability of the protein-ligand complex was also analyed using MD simulation.

The parameters of the MD Simulation like hydrogen bonds, RMSD, RMSF, Rg, etc., are also accounted in Chapter 4. Additionally, the future applications of the identified potential NLO and OL compounds and complexes were discussed in Chapter 5.

Comments:

1. **Title:** The title is appropriate and gives the basic idea about the research work carried out in the thesis.

2. **Research problem and objectives:** The research problem is well defined and the objectives of research are stated clearly. It has been also observed that the objectives of the thesis are achieved. However, the research work is diversified enough.

3. **Review of literature:** The review of literature mentioned in the thesis is relevant to the identified problem. It is clearly established in the current knowledge.

4. **Materials and methods:** The organic nonlinear optical materials selected for the present research work is clearly mentioned and the computational and experiments used in the present study are well defined. The details of density functional the DFT are also well defined to generate critical new information. The techniques used in present research work is a computer added and density functional theory including different experiments techniques like UV visible spectroscopy, solar simulator, optical limiting and fill factor etc. are appropriate.

5. **Result and discussion:** The results presented in the thesis are concise, logical, and sequential and having direct relevance to the objectives of the study. It seems that the study is a significant contribution to the existing knowledge on the non linear optical materials and its applications. The issues related to the optical materials and its properties have been discussed properly.
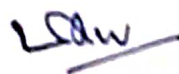
6. **Conclusion, Future Scopes and Summary:** The Conclusion and Future Scopes and Summary of the thesis have been summarised properly and the conclusion drawn are appropriate.

7. **References:** Literature cited in the present thesis is updated and well arranged.

Final Remark:

The thesis is well organized and special care has been taken in writing the contents without any ambiguity, which arises a continuous interest in the reader. The references cited in the thesis have also been presented in proper places and duly acknowledged. The work done by the candidate is a good scientific contribution with some new findings as evidenced by the good number of publications in reputed jornals and conferences attended. Publications and research work are of high quality and internationally acknowledged.

Based on the coherent presentation and publication of the work, I recommend the thesis for the award of Ph.D. degree to the candidate, subject to satisfactory performance in the viva-voce examination.

PROF. L.P. PUROHIT
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