DECLARATION

I declare that the thesis entitled **"THEORETICAL INVESTIGATION ON OPTOELECTRONIC PROPERTIES OF NANOCLUSTERS AND CONJUGATES"** has been prepared by me under the supervision of Prof. Anirban Misra, Department of Chemistry, University of North Bengal. No part of this thesis has formed the basis for the award of any degree or fellowship previously.

Tanushree Sutradhar

Tanushree Sutradhar

Department of Chemistry,
University of North Bengal,
Darjeeling-734013,
West Bengal,
India

DATE: 25.02.2021

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P.O. NORTH BENGAL UNIVERSITY, Raja Rammohunpur, Dist. Darjeeling, West Bengal, India, PIN - 734013.
PHONE : (0353) 2776 381, Fax: (0353) 2699 001

Ref. No..... *Dated.....20.....*

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I certify that the thesis entitled **"THEORETICAL INVESTIGATION ON OPTOELECTRONIC PROPERTIES OF NANOCLUSTERS AND CONJUGATES"** has been prepared by Tanushree Sutradhar, for the award of PhD degree of the University of North Bengal, under my guidance. She has carried the work at the Department of Chemistry, University of North Bengal. No part of this thesis has formed the basis for the award of any degree or fellowship previously.

25/02/2021

Prof. Anirban Misra (Supervisor)

Department of Chemistry,
University of North Bengal,
Darjeeling- 734013,
West Bengal,
India

Professor
Department of Chemistry
University of North Bengal
Darjeeling - 734013, India

DATE:

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Tanushree Sutradhar
25.02.2021

25/02/2021

Professor
Department of Chemistry
University of North Bengal
Darjeeling - 734013, India

PREFACE

For a long time we have been using optical properties to meet the urge of rapidly evolving technological world. The knowledge of the quantum chemical origin of different kinds of optical properties in organic-inorganic systems confers the idea for tuning optoelectronic material with desired functionality. We put focus to design novel fluorescent materials for the application of organic light emitting diodes (OLEDs). We have shown that electron donating and electron withdrawing groups can play a key role in tuning the fluorescent property of the conjugated organic molecule. We also put our effort to enhance the nonlinear optical (NLO) response in the designed molecular systems, as the designed systems can effectively guide the synthesis of molecules for the application of optical sensors, optical telecommunications, optical switching, optical storage etc. In continuation to design NLO material, using this charge transfer phenomena we also design organic conjugated molecules having both the photovoltaic effect for dye sensitized solar cell (DSSC) and NLO response to achieve multifunctionality in a molecules. From the urge of designing such molecules, we have proposed indole based organic conjugated molecules with varying different electron acceptor and π-linker. Simultaneous presence of these two characteristics makes the systems a promising candidate for nonlinear optics and for DSSC applications. In our study, we show that introducing zwitterionic behavior in a molecule could be a significant strategy for the amplification of NLO behavior. Inclusion of different π-linkers and electron acceptors in zwitterionic substituents has been found to have significant effect on the NLO response of molecules, where the push-pull effect in the conjugated molecules tremendously increases the hyperpolarizability values. Our next work is based on the design of efficient nanocluster functionalized NLO material. We explore that complexation of D-A groups with the BN nanocluster could be a significant strategy to design novel electro-optical BN-based material. In the final chapter, the essence of previous chapters and importance of present study has been discussed.

LIST OF TABLES

LIST OF FIGURES AND SCHEMES

APPENDICES

APPENDIX A: List of publications

PUBLISHED

1. Role of Electron-Donating and Electron-Withdrawing Groups in Tuning the Optoelectronic Properties of Difluoroboron-Napthyridine Analogues, **T. Sutradhar** and A. Misra, *J. Phys. Chem. A,* 2018, 122, 4111-4120 .

2. Enhancement of Nonlinear Optical Properties of Indole Based Dyes through Electron Acceptor and π-Linker for Dye-Sensitized Solar Cell Applications, **T. Sutradhar** and A. Misra, *ChemistrySelect ,* 2019, *4,* 3697 –3705 .

3. The Role of π -Linkers and Electron Acceptors in Tuning the Nonlinear Optical Properties of Bodipy based Zwitterionic Molecules, **T. Sutradhar** and A. Misra, RSC Adv., 2020, 10, 40300–40309.

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4. A Theoretical Study on the Nonlinear Optical Property of Boron Nitride Nanoclusters Functionalized by Electron Donating and Electron Accepting Groups, **T. Sutradhar** and A. Misra, Communicated, **2020**.

APPENDIX B: Oral and poster presentations

Oral Presentation

1. Role of Electron-Donating and Electron-Withdrawing Groups in Tuning the Optoelectronic Properties of Difluoroboron-Napthyridine Analogues, **Tanushree Sutradhar** and Anirban Misra*, National Seminar on "Frontiers in Chemistry 2017-18", Organized by Department of Chemistry, University of North Bengal, Darjeeling, India.

Poster Presentation

2. Role of Electron-Donating and Electron-Withdrawing Groups in Tuning the Optoelectronic Properties of Difluoroboron-Napthyridine Analogues, **Tanushree Sutradhar** and Anirban Misra*, National Seminar on "19th CRSI National Symposium in Chemistry, July 2016", Organized by Department of Chemistry, University of North Bengal, Darjeeling, India.

3. Enhancement of Nonlinear Optical Properties of Indole Based Dyes through Electron Acceptor and π-Linker for Dye-Sensitized Solar Cell Applications, **Tanushree Sutradhar** and Anirban Misra*, International Seminar on "Frontiers in Chemistry 2018", Organized by Department of Chemistry, University of North Bengal, Darjeeling, India.

APPENDIX C: Acknowledgement

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Darjeeling Tanushree Sutradhar
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