

DECLARATION

I declare that the thesis entitled "THEORETICAL INVESTIGATION ON OPTOELECTRONIC PROPERTIES OF NANOCCLUSERS 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.

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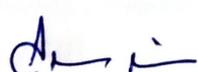
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I certify that the thesis entitled "THEORETICAL INVESTIGATION ON OPTOELECTRONIC PROPERTIES OF NANOCCLUSERS AND CONJUGATES" has been prepared by Tanushree Sutradhar, for the award of PhD degree of the University of North Bengal, under my guidance. She 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.

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69

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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

Table	Caption	Page
Table 1.3.1.	Susceptibility functions ($\chi^{(2)}$ and $\chi^{(3)}$) for various types for interacting field components, their effects and applications.	19
Table 3.1.	Calculated maximum absorption wavelengths (in nm), the oscillator strength (f), orbital contribution, and excitation energies (in eV) with TD-B3LYP/6-311+G (d) for difluoroboron naphthyridine molecule in gas phase and in dichloromethane solvent (DCM).	59
Table 3.2.	Calculated emission wavelength (in nm) (electronic transition $S_1 \rightarrow S_0$), the oscillator strength (f), orbital contribution, and emission energies (in eV) of difluoroboron naphthyridine molecule at the TD-B3LYP/6-311+G (d) level of theory.	63
Table 3.3.	Calculated ionization potentials (IPs in eV), electron affinities (EAs in eV), reorganization energies (eV) for hole (λ_{hole}) and electron ($\lambda_{\text{electron}}$) of the BF ₂ -naphthyridine molecules (A to E). Calculations are done by applying adiabatic condition.	67
Table 4.1.	Main electronic transitions, oscillator strength and light harvesting efficiency of indole-based dyes in gas phase at CAM-B3LYP/6-311++G(d,p) level of theory.	83
Table 4.2.	The dipole moment, static polarizability, first and second order hyperpolarizability of dyes studied at the B3LYP/6-311+G(d,p) level of theory in gas phase.	86
Table 4.3.	E^{dye^*} and E^{dye} is excited state and ground state oxidation potentials, E_{0-0} represents electronic vertical transition energy, ΔG_{inject} is electron injection free enthalpy, E_b denotes excitation binding energy and eV_{OC} represents open circuit voltage of the studied dyes at the B3LYP/6-311++G(d,p) level of theory in gas phase.	87
Table 4.4.	Calculated ionization potentials (IP), electron affinities (EA), reorganization energies (λ_{hole} and $\lambda_{\text{electron}}$), chemical potential ($\mu_{\text{c.p}}$), chemical hardness (η) and softness (s) of the dyes in gas phase at the B3LYP/6-311++G(d,p) level of theory.	88
Table 5.1.	Dipole moment (μ), static polarizability ($\Delta\alpha$) and $\mu\beta$ of the studied dyes at the B3LYP/6-311++G (d,p) level of theory.	103

Table 5.2.	β_x , β_y , and β_z components (10^{-30} esu) of studied molecules (1 to 2d) obtained from DFT calculation (B3LYP functional), employing the 6-311++G(d,p) basis set.	106
Table 5.3.	Major transition energy, Δr index, integral overlap of hole electron distribution (s) and distance between centroid of hole and electron (D) calculated at CAM-B3LYP/6-311++G (d,p) level of theory.	107
Table 5.4.	TDDFT benchmarking of theoretical and experimental maximum absorption wavelength (λ_{\max}), f represents oscillator strength.	109
Table 5.5.	Main electronic transitions, maximum absorption wavelength (λ_{\max}), oscillator strength (f) and transition nature of BODIPY based dyes in gas phase at CAM-B3LYP/6-311++G (d,p) level of theory.	110
Table 5.6.	Calculated ionization potentials (IP), electron affinities (EA), reorganization energies (λ_{hole} and $\lambda_{\text{electron}}$) of the dyes in gas phase at the B3LYP/6-311++G(d,p) level of theory (in eV).	111
Table 6.1.	Bond lengths, dihedral angles and bond angles of electron donating and accepting group functionalized $B_{12}N_{12}$ nanoclusters (1a to 3f)	126
Table 6.2.	Dipole moment (μ), adsorption energy (E_{ads}), HOMO-LUMO gap (E_g) of the studied systems at the B3LYP/6-31+G(d) level of theory.	134
Table 6.3.	Hyperpolarizability values ($\times 10^{-30}$ esu) of studied molecules obtained from DFT calculation (CAMB3LYP functional), employing the 6-311+G(d) basis set.	138
Table 6.4.	Major transition energy, Δr index, integral overlap of hole electron distribution (s) and distance between centroid of hole and electron (D) calculated at CAM-B3LYP/6-311+G(d) level of theory.	139
Table 6.5.	Main electronic transitions, maximum absorption wavelength (λ_{\max}), oscillator strength (f) and transition nature of donor-acceptor decorated $B_{12}N_{12}$ cluster in gas phase at B3LYP/6-311++G(d,p) level of theory.	141

LIST OF FIGURES AND SCHEMES

Figure & Scheme	Caption	Page
Figure 1.2.1.	Classification of luminescence based on duration of emission	4
Figure 1.2.2.	Jablonski diagram representing the absorption, fluorescence and phosphorescence.	6
Figure 1.2.3.	Stokes shift and the mirror image rule	8
Figure 1.2.4.	Fluorescence lifetime decay profile	8
Figure 1.2.5.	Fluorophore-solvent excited state interactions.	9
Figure 1.3.1.	Linear and nonlinear interactions of waves and the media.	11
Figure 1.3.2.	Energy band diagram of linear (left) and nonlinear optics (right).	12
Figure 1.3.3.	(a) Polarization response (P) plot to an incident electromagnetic wave of field strength $E(\omega)$ in a noncentrosymmetric medium at frequency ω . (b) to (d) Fourier components of P at frequencies 2ω , ω , and 0.	14
Figure 1.3.4.	Nonlinear polarization response (P) plot to an incident electromagnetic field in a centrosymmetric medium.	15
Figure 1.3.5.	Model system with electron donor and acceptor substituents which results the asymmetric charge distribution along with high β . According to the reference coordinate system z-axis is parallel to the dipolar axis of the molecule, the molecule polarized easily along z direction. Hence β_{zzz} is the largest component of the β_{ijk} tensor.	16
Figure 1.3.6.	Second harmonic generation (SHG) process.	17
Figure 1.3.7.	Paramagnetic generation.	18
Figure 1.4.1.	Diagram of solar cell.	23
Figure 1.4.2.	Construction of the dye-sensitized solar cells.	24
Figure 2.4.1	Working Principle of dye-sensitized solar cells	44
Figure 3.1.	Proposed structure of naphthyridine fused difluoroboron compounds. Blue color denotes N ⁺ C ⁻ O moiety.	52
Figure 3.2.	Selected bond parameters obtained from the optimized geometries of BF ₂ -naphthyridine derivatives. Note: φ indicates dihedral angles ($\varphi_1 = \text{C11-C10-C13-C14}$; $\varphi_2 = \text{C11-C10-C15-C16}$; $\varphi_3 = \text{C11-C10-C13-C14}$, $\varphi_4 = \text{C10-C11-C16-C17}$; $\varphi_5 = \text{C7-C8-C13-C14}$); and θ indicates bond angles ($\theta_1 = \text{C13-C14-H}$, $\theta_2 = \text{C15-C16-F}$, $\theta_3 = \text{C13-C14-CHO}$, $\theta_4 = \text{C16-C17-CH}_3$, $\theta_5 =$	55

	C13–C14–NH ₂). Brown color denotes parameters of the ground state and black color depicts parameters of the excited state. All data provided in the figure are in gas phase.	
Figure 3.3.	Computed absorption spectra (a) in gas phase and (b) in DCM recorded with TD-B3LYP/6-311 + G (d).	58
Figure 3.4.	Computed emission spectra with TD-B3LYP/6-311+ G (d) (a) in gas phase and (b) in dichloromethane solvent (DCM) of difluoroboron naphthyridine molecule.	62
Figure 3.5.	Frontier Molecular Orbital (FMO) energy level diagram of the difluoroboron naphthyridine molecules in gas phase and in dichloromethane solvent (DCM).	65
Figure 3.6.	Frontier molecular orbitals of the molecule BF ₂ - naphthyridine derivative (E) in gas phase (left panel) and in DCM (right panel).	65
Figure 4.1.	Schematic energy level diagrams of the dyes in gas phase, the CB of TiO ₂ , and the electrolyte (I ⁻ /I ₃ ⁻).	80
Figure 4.2.	Composition of frontier molecular orbitals (FMO) of various fragments of the indole based dyes (A) Different fragments involved in the calculation of percentage contribution to FMOs. (B) FMO composition (%).	81
Figure 4.3	First order hyperpolarizability of indole based dyes studied at the B3LYP/6-311++G (d,p) level of theory in gas phase.	86
Figure 5.1.	Chemical structures of the BODIPY-based dyes under investigation.	97
Figure 5.2.	Energy level diagrams of the dyes in gas phase at B3LYP/6-311++G (d,p) level of theory.	100
Figure 5.3.	Frontier molecular orbitals of the dyes in the gas phase at B3LYP/6-311++G (d,p) level of theory.	102
Figure 5.4.	First hyperpolarizability of BODIPY based dyes studied at B3LYP/6-311++G (d,p) level of theory.	104
Figure 5.5	The transition dipole moment density of the studied molecules (1 to 2d). Isovalue is 2×10^{-4} . The green colour implies charge increase upon excitation and the blue colour implies charge depletion.	107
Figure 6.1.1	Bond lengths between the B ₁₂ N ₁₂ cluster and donor-acceptor groups at B3LYP/6-31+G(d) level of theory.	125
Figure 6.1.2	Optimized structure of B ₁₂ N ₁₂ , 1a, 1c, 1d and 1f.	126
Figure 6.1.3	Optimized structure of 2a to 2f.	128
Figure 6.1.4	Optimized structure of 3a to 3f.	131
Figure 6.2.	Frontier molecular orbitals of the donor-acceptor decorated B ₁₂ N ₁₂ cluster at B3LYP/6-31+G(d) level of theory.	135
Figure 6.3.	MEP plots of the B ₁₂ N ₁₂ , 1f, 2f and 3f nanoclusters. To understanding the colors in these figures, the reader must read the web version of this article. The isosurface value is $0.0004 \text{ e}/\text{\AA}^3$.	136
Figure 6.4.	The transition dipole moment density of the designed clusters. Isovalue is 2×10^{-4} . The green and blue isosurface indicates positive and negative contributions.	140

Scheme 1.3.1.	P-nitroaniline dimethylaminonitrisostilbene molecules, the prototypical dipolar D- π -A system.	19
Scheme 1.3.2.	Dipolar <i>vs.</i> octupolar charge distribution in prototypical dipolar and trigonal octupolar systems.	20
Scheme 3.1.	Basic types of difluoroboranyl complexes.	50
Scheme 4.1.	Chemical structures of the indole-based dyes.	75
Scheme 6.1.	Chemical structures of electron donating and accepting group functionalized B ₁₂ N ₁₂ nanoclusters.	118

APPENDICES

APPENDIX A: List of publications

PUBLISHED

1. Role of Electron-Donating and Electron-Withdrawing Groups in Tuning the Optoelectronic Properties of Difluoroboron-Naphthyridine 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.

COMMUNICATED

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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