

TABLE OF CONTENTS

Chapter 1: Optical properties of organic conjugated compounds and nanoclusters

1-31

1.1. Introduction	2
1.2. Luminescence	3
1.2.1. Classification of luminescence	3
1.2.2. Types of luminescence	4
1.2.3. Basic principles of luminescence	5
1.2.4. Fluorescence	6
1.2.5. Stokes shift and the mirror image rule	7
1.2.6. Fluorescence lifetime	8
1.2.7. Solvent effects on fluorescence emission	9
1.3. Nonlinear Optical Property	10
1.3.1. Definition of nonlinear optics	10
1.3.2. Origin of NLO	12
1.3.3. Microscopic nonlinearities	15
1.3.4. Various types of second order NLO effects	16
1.3.4.1. Second harmonic generation (SHG)	16
1.3.4.2. Sum frequency generation or parametric generation	17
1.3.4.3. Linear electrooptic effect or pockels effect	18
1.3.4.4. Optical rectification	18
1.3.5. Applications of NLO effects	18
1.3.6. Present status of the field	19
1.3.6.1. Organic molecules for second-order nonlinear optics	20
1.3.6.2. Nanocluster complexes for second-order nonlinear optics	22
1.4. Photovoltaic Property	22
1.4.1. Recent technology: Semiconductor solar cell	23
1.4.2. Dye sensitized solar cells	24
1.4.3. Titanium dioxide	25
1.4.4. Dye molecules	25
1.4.5. Electronic and optical properties of isolated dyes	26
1.4.6. Organic dyes	26
1.4.7. Present status of the field	27
1.5. Aim of the present work	27
1.6. References	29

2.1. Theoretical Determination of Fluorescence	33
2.1.1. Spectroscopic transition strengths	33
2.1.2. Einstein coefficients	34
2.1.3. Radiative rate constant	35
2.1.4. Fluorescence quantum yield	36
2.1.5. Fluorescence lifetime	36
2.1.6. Solvatochromism	37
2.2. Theoretical determination of first hyperpolarizability (β)	38
2.2.1. Early models for the calculation of β	38
2.2.1.1. Equivalent field model (EIF)	38
2.2.1.2. Additivity model	39
2.2.1.3. Two-state model	39
2.3. Quantum chemical calculation for the calculation of NLO response	40
2.3.1. Sum over states (SOS) methods	40
2.3.2. Coupled perturbed Hartree Fock (CPHF) methods	41
2.4. Theoretical determination of Dye-Sensitized Solar Cells (DSSSC)	43
2.4.1. Working Principle of Dye-Sensitized Solar Cells	43
2.4.2. Photovoltaic properties of dye sensitized Solar cell (DSSC)	44
2.4.3. Electron injection	46
2.4.4. Open circuit photovoltage (V_{oc})	46
2.5. References	47

3.1. Introduction	50
3.2. Computational Details	52
3.3. Results and Discussions	53
3.3.1. Structural parameters	53
3.3.2. Effect of solvent polarity in the dipole moment	56
3.3.3. Absorption properties	56

3.3.4.	Emission spectra	60
3.3.5.	Frontier molecular orbitals	63
3.3.6.	Ionization potential and electron affinity	66
3.3.7.	Reorganization energy	67
3.4.	Conclusions	68
3.5	References	69
 <i>Chapter 4: Enhancement of nonlinear optical properties of indole based dyes through electron acceptor and π-linker for dye-sensitized solar cell applications</i>		 72-93
4.1.	Introduction	73
4.2.	Theoretical Background	75
4.2.1.	Nonlinear optical properties (NLO)	75
4.2.2.	Photovoltaic properties of dye sensitized Solar cell (DSSC)	76
4.3.	Computational Details	77
4.4.	Results and Discussions	78
4.4.1.	Geometrical structures	78
4.4.2.	Frontier molecular orbitals	78
4.4.3.	Electron transfer process	81
4.4.4.	Absorption properties	82
4.4.5.	Dipole moment	83
4.4.6.	Nonlinear optical properties	84
4.4.7.	Photovoltaic properties	86
4.4.8.	Ionization potential, electron affinity and reorganization energy	88
4.5.	Conclusion	89
4.6.	References	90
 <i>Chapter 5: The role of π-linkers and electron acceptors in tuning the nonlinear optical properties of BODIPY based zwitterionic molecules</i>		 94-116
5.1.	Introduction	95

5.2. Theoretical Background and Computational Details	97
5.3. Results and discussions	99
5.3.1. Electronic structure	99
5.3.2. NLO properties	102
5.3.3. UV-VIS spectra of dyes	108
5.3.4. Ionization potential, electron affinity and reorganization energy	110
5.4. Conclusions	112
5.5. References	113
<i><u>Chapter 6: A theoretical study on the nonlinear optical property of boron nitride nanoclusters functionalized by electron donating and electron accepting groups</u></i>	117-145
6.1. Introduction	118
6.2. Theoretical Background and Computational Details	121
6.3. Results and discussions	122
6.3.1. Structural parameters	122
6.3.2. Dipole moment	135
6.3.3. Molecular electrostatic potential (MEP) analysis	136
6.3.4. Nonlinear optical properties	137
6.3.5. Absorption properties	141
6.4. Conclusions	143
6.5. References	144
<i><u>Chapter 7: General conclusion</u></i>	146-150
<i><u>Bibliography</u></i>	151-164
<i><u>Index</u></i>	165-166