CHAPTER 1: GENERAL INTRODUCTION
1.1 Introduction.................................................................................................................................................. 2
1.2 Electronic spectroscopy and Photo-physics.................................................................................................. 5
    1.2.1 Relaxation Processes in excited state
        a) Photo-Physical Relaxation Processes
        b) Photo-chemical Relaxation Processes:
1.3 The absorption process (Beer-Lambert law). ......................................................................................... 7
    1.3.1 Electronic transition in molecular absorption
        a) σ→σ* Transitions:
        b) n→σ* Transitions
        c) n→π* transitions
        d) π→π* transitions
    1.3.2 Symmetry-forbidden transitions
        a) Vibronic Coupling
1.4 Fluorescence.................................................................................................................................................. 14
    1.4.1 Stokes shift
    1.4.2 Lifetime
    1.4.3 Quantum Yield
    1.4.4 Polarization
1.5 Circular Dichroism and Optical Rotatory Dispersion.............................................................................. 17
1.6 Near field effect on photo-physics.............................................................................................................. 21
    1.6.1 Metal enhanced Emission
    1.6.2 Surface Plasmon Coupled Emission
1.7 Solvent Interaction………………………………………………………………………………23
  a) Solvent Relaxation
  b) Hydrogen Bonding Solvent Effect
  c) Reversal of Excited Emission Levels
  d) Edge Excitation Red Shift (EERS)

CHAPTER 2: METHODOLOGY: EXPERIMENTAL TECHNIQUES AND
COMPUTATIONAL SIMULATION

2.1 Introduction……………………………………………………………………………..32

2.2 Experimental techniques……………………………………………………………………32
  2.2.1 Sample preparation
  2.2.2 Steady state measurements
    2.2.2. (a) Steady state Absorption measurements
    2.2.2. (b) Steady State Fluorescence and Excitation Measurements
      (i) Continuous Light Source (Xenon Lamp)
      (ii) Monochromators
      (iii) Sample Chamber
      (iv) Detector
    2.2.2 (c) Time Resolved Measurements
      (i) Data Analysis
      (ii) Precautions and Sources of Error in TCSPC
    2.2.2 (d) Vacuum coating unit
    2.2.2 (e) X-ray photoelectron spectroscopy (XPS) Measurements

2.3 Computational spectroscopy and Electronic structure Calculations………………….46
  2.3.1 Density Functional Theory
  2.3.2 Time Dependent Density Functional Theory (TD-DFT)
  2.3.3 (a) Basis sets and Basis Function
  2.3.3 (b) Minimal basis set
  2.3.3 (c) Split valence basis set
2.3.3 (d) Polarization and diffusion functions

2.3.4 Molecular Properties

(a) Molecular Geometry
(b) Dipole Moment
(c) Molecular electrostatic potential surfaces
(d) Frontier molecular orbital (FMO)
(e) Frequency

2.3.5 Electronic spectra

2.3.6 Vibrationally-Resolved Electronic (Vibronic) spectra

(a) Vibronic Absorption Spectra
(b) Vibronic Emission Spectra
(c) Electronic Circular Dichroism

Chapter 3: ELECTRONIC AND VIBRONIC STRUCTURAL STUDIES AND PHOTOPHYSICS OF PROTONATION OF QUINOLINE.

3.1 Introduction................................................................................................................. 58

3.2 Methods..................................................................................................................... 61

3.2.1 Computational details
3.2.2 Experimental Techniques

3.3 Result and Discussion................................................................................................. 63

3.3.1 Steady state absorption and fluorescence measurements
3.3.2 Time domain fluorescence measurements

3.3.3 (i) Ground State optimizations
3.3.3 (ii) Molecular electrostatic potential (MEP) map at ground state
3.3.3 (iii) Conceptual-DFT Based global reactivity descriptors

3.3.4 Electronic absorption and emission transition Studies
3.3.5 Vibronic absorption and emission Studies
3.3.6 Ground and Excited State vibrational structure Studies

3.3.6 (a) Vibrations due to aromatic residues
3.3.6 (b) Vibrations due to the presence of heteroatom

3.3.7 Excitation and Absorption spectra, Revisited

3.4 Conclusion .................................................................................................................. 83

CHAPTER 4: EFFECT OF ELECTRIC FIELD ON PHOTO-PHYSICS OF QUINOLINE

4.1 Introduction .................................................................................................................. 86
4.2 Theory .......................................................................................................................... 89
4.3 Computational details ............................................................................................... 91
4.4 Result and Discussion ............................................................................................... 92
    4.4.1 Electro absorption (EA) electronic structure calculations
    4.4.2 Electro-emission (E-PL) from electronic structure calculations
4.5 Conclusion .................................................................................................................. 105

Chapter 5: NEAR FIELD EFFECT OF SILVER NANOPARTICLES ON THE PHOTO-PHYSICS OF QUININE SULPHATE AND ITS DI-CATION DOPED IN POLYVINYL ALCOHOL THIN FILM

5.1 Introduction .................................................................................................................. 108
5.2 Experimental Section ............................................................................................... 111
    5.2.1 Materials
    5.2.2 Silver Nano-Islands Film (SNIF) Formation
    5.2.3 Instrumentation
5.3 Results and Discussions ........................................................................................... 113
    5.3.1 Steady state absorption and Fluorescence measurements
    5.3.2 Time Domain fluorescence measurements
    5.3.3 Edge Excitation Red Shifted Emission (EERS) spectral Measurements
    5.3.4 Photostability Measurements
5.4 Conclusion .................................................................................................................. 123
CHAPTER 6: PHOTOPHYSICS OF 5-AMINOQUINOLINE IN ACETONITRILE: WATER BINARY SOLVENT MIXTURE: REVISITED

6.1 Introduction……………………………………………………………………………………………………… 125
6.2 Methodology………………………………………………………………………………………………………… 129
   6.2.1 Experimental Section
   6.2.2 Computational Detail
6.3 Results and Discussion…………………………………………………………………………………………… 130
   6.3.1 Steady state measurements
   6.3.2 Time Domain Measurements
   6.3.3 Electronic structure calculations
6.5 conclusion…………………………………………………………………………………………………………… 142

Bibliography

List of Publications
Copies of the Reprints of the Published Papers
Personal Profile (BIO-DATA)