

CONTENTS

	Page
Acknowledgement	c
Abstract in Thai	d
Abstract in English	f
List of Tables	k
List of Figures	m
List of Abbreviations	p
List of Symbols	q
Statements of Originality in Thai	s
Statements of Originality in English	t
Chapter 1 Introduction	
1.1 Classical Detection	1
1.2 Sensing Technology	2
1.2.1 Physical Sensors	2
1.2.2 Chemical Sensors	2
1.2.3 Biosensors	4
1.3 Photoluminescence Concept	5
1.3.1 Principle of Photoluminescence	5
1.3.2 Excited-State Intramolecular Proton Transfer	6
1.3.3 Application and Instrumental Devices	7
1.4 Derivatives of 2-(2'-Hydroxyphenyl)benzimidazole	10
1.5 Derivatives of 2-(2'-Aminophenyl)benzothiazole	14
1.6 Research Objectives	16
Chapter 2 Theoretical and Computational Details	
2.1 Density Functional Theory	19

2.1.1	The Hohenberg-Kohn Theorem	19
2.1.2	Kohn Sham Equation	20
2.1.3	Hybrid Functionals	20
2.1.4	Long-Range Corrected Hybrid Functionals	22
2.1.5	Basis Set	23
2.2	Time-Dependent Density Functional Theory	24
2.3	Molecular Orbitals of Benzene Derivatives	25
Chapter 3	Heteroatom Effect on Photophysical Properties of 2-(2'-Hydroxyphenyl)benzimidazole and Its Derivatives as Fluorescent Dyes: a TD-DFT Study	
3.1	Introduction	26
3.2	Computational Details	30
3.3	Results and Discussions	32
3.3.1	The Effect of DFT Functionals	32
3.3.2	Ground State Optimization and Structural Parameter of HBX Derivatives	34
3.3.3	Calculated Absorption Spectra of HBX Derivatives	34
3.3.4	Frontier Molecular Orbitals and Energy Band Gap of HBX Derivatives	37
3.3.5	Emission Spectra of Selected Derivatives	45
3.3.6	Calculated IR Spectra of the Ground and Excited State of Selected Derivatives	46
3.3.7	Potential Energy Curves of the Ground and Excited State	49
3.4	Chapter Summary	50
Chapter 4	TD-DFT Study of Absorption and Emission Spectra of 2-(2-Aminophenyl)benzothiazole Derivatives in Water	
4.1	Introduction	52

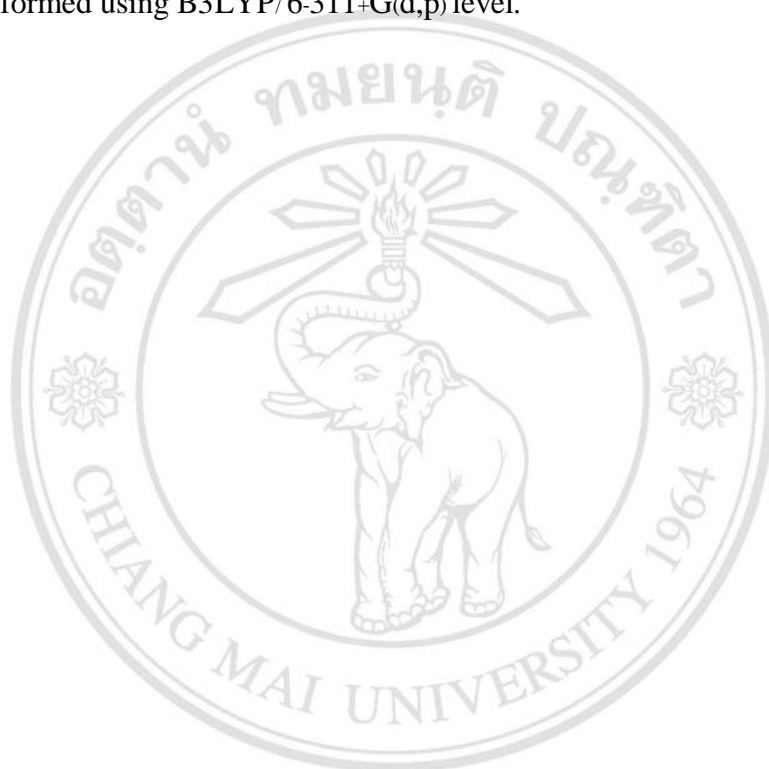
4.2	Computational Details	54
4.3	Results and Discussions	56
4.3.1	Exchange-Correlation Functional Selection	56
4.3.2	Ground and Excited States of APBT and Its Derivatives	57
4.3.3	Absorption and Energy Band Gap of APBT Derivatives	58
4.3.4	Emission Spectra and Stokes' Shift	61
4.3.5	Potential Energy Curves of Proton Transfer	66
4.4	Chapter Summary	67
Chapter 5	Conclusions	68
	References	70
	List of Publications	80
	Appendix A Conferences and Workshops	81
	Appendix B Publications and Posters	82
	Curriculum Vitae	86

ลิขสิทธิ์มหาวิทยาลัยเชียงใหม่
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LIST OF TABLES

Table	Page
2.1 Spitting scheme of 6-311G(d,p) basis set.	23
3.1 Maximum wavelength (λ_{\max}) of first excitation and deviation between the calculated and experimental wavelengths ($\Delta\lambda$) for HBI calculated by various TD-DFT methods with 6-311+G(d,p) basis set.	33
3.2 The selected bond lengths (\AA) and dihedral angles (degree) for ground state optimized structures calculated by B3LYP/6-311+G(d,p) level of theory.	34
3.3 Calculated maximum wavelengths of absorption spectra of enol form (nm), excitation energies (eV), oscillator strengths (f) and major contributions (%) of HBX and derivatives. The calculations were performed using TD-B3LYP/6-311+G(d,p) level.	38
3.4 Keto emission wavelengths (nm), excitation energy (eV), oscillator strength (f) and major contributions (%) for selected derivatives of HBI, HBO and HBT. The calculations were performed using TD-B3LYP/6-311+G(d,p) level.	46
3.5 The lengths of hydrogen bond (\AA) of N–H and O–H of HBX derivatives for ground and excited state optimized structures calculated by B3LYP/6-311+G(d,p) level of theory.	48
4.1 Available experimental absorption wavelengths compared to theoretical simulations for APBT and APBT04 in solution phase using different density functional theory (DFT) methods with hybrid exchange functional at 6-311+G(d,p) basis set.	56
4.2 The selected bond lengths (\AA) and dihedral angles (degree) for ground and excited state optimised structures calculated by B3LYP/6-311+G(d,p) level of theory.	57

- 4.3 Absorption wavelengths (nm), excitation energy (eV), oscillator strength (f) and major contributions (%) of APBT derivatives in water. The calculations were performed using B3LYP/6-311+G(d,p) level. 60
- 4.4 Emission wavelengths (nm), excitation energy (eV), oscillator strength (f) and major contributions (%) of APBT and its derivatives in water. The calculations were performed using B3LYP/6-311+G(d,p) level. 63



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LIST OF FIGURES

Figure	Page
1.1 Physical properties to electrical energy of physical sensors.	2
1.2 Principle of fluorescent sensor. (a) “OFF” and (b) “ON” signals of fluorescence.	3
1.3 An ‘OFF–ON’ fluorescent chemosensor based on rhodamine6G-2-chloronicotinaldehyde (R6CN) for the detection of Al ³⁺ ions	3
1.4 Schematic representation of component of biosensor.	4
1.5 (a) The schematic representation of glucose sensors. (b) the reaction mechanism of the glucose oxidase enzyme in glucose sensors.	5
1.6 Jablonski diagram describing light absorption and emission processes.	6
1.7 The photocycle of excited-state intramolecular proton transfer.	7
1.8 The molecular structure of some fluorophore.	8
1.9 Some molecules as fluorescent probe for detect biothiols (a), reactive oxygen species (b) and metal ions such as Zn ²⁺ (c).	9
1.10 The Organic Light Emitting Diode (OLED) structure.	10
1.11 Reaction mechanism of Van Leusen imidazole synthesis.	11
1.12 Reaction mechanism of benzimidazole synthesis.	11
1.13 Reaction of 2-(2'-Hydroxyphenyl)benzimidazole (HBI) synthesis.	11
1.14 The molecular structure of (a) 2-(2'-Hydroxyphenyl)benzoxazole; HBO and (b) 2-(2'-Hydroxyphenyl)benzothiazole; HBT.	13
1.15 The reaction mechanism of azido to amine of APBT proposed by quantum mechanical calculations.	15
2.1 Basic concept for the Density Functional Theory.	19

2.2	The molecular orbital of Benzene (a) and Pyridine (b).	25
3.1	Excited-State Intramolecular Proton Transfer (ESIPT) of the HBX molecules (where X = NH, O and S, respectively). S_0 is the ground state and S_1 is the first lowest excited-state. E is enol form and K is keto form.	27
3.2	Molecular structures of HBX derivatives, where X = NH, O and S namely 2-(2'-hydroxyphenyl)benzimidazole (HBI), 2-(2'-hydroxyphenyl)-benzoxazole (HBO) and 2-(2'-hydroxyphenyl)benzothiazole (HBT), respectively. Numbers 1-8 represent the substitution position by substituents and hetero nitrogen atoms.	28
3.3	Molecular structures of HBX molecules. 1, 2, 3 and 4 indicate the substitution positions by hetero nitrogen atom used in this work.	31
3.4	Calculated absorption spectra of HBI by various TD-DFT methods with hybrid exchange functional at 6-311+G(d,p) basis set.	33
3.5	Calculated absorption spectra of (a) HBI, (b) HBO, (c) HBT and their derivatives in water. The calculations were performed using TD-B3LYP/6-311+G(d,p) level.	35
3.6	Frontier molecular orbitals of selected derivatives of HBX computed at B3LYP/6-311+G(d,p) level.	39
3.7	Frontier molecular orbitals of enol HBI and its derivatives computed at B3LYP/6-311+G(d,p) level.	40
3.8	Frontier molecular orbitals of enol HBO and its derivatives computed at B3LYP/6-311+G(d,p) level.	41
3.9	Frontier molecular orbitals of enol HBT and its derivatives computed at B3LYP/6-311+G(d,p) level.	42
3.10	Density difference plot for selected derivatives of HBX computed at B3LYP/6-311+G(d,p) level. (isovalue = 0.0200 a.u.)	43
3.11	Diagram of calculated HOMO and LUMO energy levels and HOMO-	44

	LUMO gaps (eV) at B3LYP/6-311+G(d,p) level of enol absorption of (a) HBI, (b) HBO and (c) HBT and their derivatives.	
3.12	Calculated enol absorption (blue line) and keto emission (red line) spectra of selected HBX derivatives obtained from TD-B3LYP/6-311+G(d,p) level.	45
3.13	Calculated IR spectra of ground (blue line) and excited state (red line) of selected derivatives of HBI, HBO and HBT in the spectral region of O–H stretching mode calculated at the B3LYP/6-311+G(d,p) level.	47
3.14	Potential energy curves of ground and excited states for selected derivatives of HBX and their derivatives with O–H bond length. The insert shows the corresponding optimized geometries.	50
4.1	Molecular structures of 2-(2'-Aminophenyl)benzothiazoles (APBT) and its derivatives. R ₁ , R ₂ and R ₃ indicate the substitution positions used in this work.	55
4.2	Calculated HOMOLUMO energy level diagram of APBT and its derivatives obtained from B3LYP/6-311+G(d,p) level.	59
4.3	Frontier HOMO and LUMO molecular orbitals of APBT and its derivatives obtained from B3LYP/6-311+G(d,p) level.	62
4.4	Simulated absorption (blue dashed line) and emission (red solid line) spectra of APBT and its derivatives by TD-B3LYP/6-311+G(d,p) in water.	65
4.5	Potential energy curves of ground and excited states for selected derivatives with N–H bond length. The insert shows the corresponding optimized geometries.	66

LIST OF ABBREVIATIONS

IC	Internal conversion
ISC	Intersystem crossing
BODIPY	Boron-dipyrromethene
ESIPT	Excited-state intramolecular proton transfer
HBI	2-(2'-Hydroxyphenyl)benzimidazole
HBO	2-(2'-Hydroxyphenyl)benzoxazole
HBT	2-(2'-Hydroxyphenyl)benzothiazole
nm	Nanometer
HF	Hartree-Fock approximation
CPCM	The nonequilibrium polarizable continuum model calculations
DFT	Density functional theory
B3LYP	Becke, 3-parameter, Lee-Yang-Parr exchange-correlation functional
PBE0	Perdew, Burke, and Ernzerhof exchange-correlation functional
CAM-B3LYP	Handy and coworkers' long-range corrected version of B3LYP using the Coulomb-attenuating method
ω B97XD	Functional from Head-Gordon and coworkers including empirical dispersion
LC-BLYP	The long correction of Hirao and coworkers
TD-DFT	Time-dependent density functional theory
HOMO	Highest occupied molecular orbital
LUMO	Lowest unoccupied molecular orbital
kcal·mol ⁻¹	Kilocalorie per mole
eV	Electron volts
ICT	Intramolecular charge transfer
PECs	Potential Energy Curves

APBT 2-(2'-Aminophenyl)benzothiazole

AzPBT 2-(2'-Azidophenyl)benzothiazole



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LIST OF SYMBOLS

S	Excited singlet state
T	Excited triplet state
ν	Frequency
S_0	Ground state
S_1	First excited singlet state
S_2	Second excited singlet state
T_1	First excited triplet state
$^\circ$	Degree
R	Substituent
Ψ	Wavefunction
\hat{H}	Hamiltonian operator
E	Total energy
ψ	Wavefunction associated with solving the electron part
χ	Wavefunction associated with nuclear motion
T	Kinetic energy
V	Potential energy
$T_N(R)$	Kinetic energy of the nuclei
$T_e(r)$	Kinetic energy of the electrons
$V_{eN}(r, R)$	Electron-nuclei attractive Coulomb potential
$V_{NN}(R)$	Nuclear-nuclear repulsive Coulomb potential and
$V_{ee}(r)$	Electron-electron repulsive Coulomb potential
N	Many electron
$\psi_i(N)$	Spin-orbital
\hat{f}	Fock operator
ε_i	Spin-orbital energy
$\hat{H}^{(0)}$	Unperturbed Hamiltonian

∞	Infinity
ρ	Electron probability density
$\rho(r)$	Entire electron density of the molecule
$E[\rho]$	Electronic energy as a function of electron density
$E_T[\rho]$	Kinetic energy as a function of electron density
$E_V[\rho]$	Potential energy as a function of electron density
$E_U[\rho]$	External energy as a function of electron density
$E_{XC}[\rho]$	Exchange-correlation energy as a function of electron density
V_{XC}	Exchange-correlation potential
$\delta\rho$	Integral of electron density
$E_{XC}^{Hybrid}[\rho]$	Hybrid functional energy of a mixture of Hartree-Fock exchange with DFT exchange-correlation
C	Constants determined by Becke
$\rho(r, t)$	Time-dependent potentials and electron densities
s	s -orbital
p	p -orbital
d	d -orbital
π	Pi
$\pi\pi^*$ and $\pi-\pi^*$	Pi to pi* transition (proton transfer)
$n\pi^*$ and $n-\pi^*$	n to Pi* transition (intramolecular charge transfer)
\AA	Angstrom
ΔE	Relative energy
%	Percent
f	Oscillator strength
$\Delta\lambda$	Deviation between the calculated and experimental wavelength

ข้อความแห่งการริเริ่ม

- 1) การออกแบบโมเลกุลสี่ข้อมฟลูออเรสเซนต์ตัวใหม่โดยวิธีการทางเคมีคอมพิวเตอร์ซึ่งเป็นมิตรต่อสิ่งแวดล้อม ปราศจากสารเคมีที่เป็นพิษ ประหยัดเวลาและเป็นแนวทางสำคัญในกระบวนการสังเคราะห์แก่นักเคมี
- 2) การศึกษาสมบัติแสงเชิงฟิสิกส์และแสงเชิงเคมีของสี่ข้อมฟลูออเรสเซนต์โดยการเติมเฮเทอโรอะตอมหรือหมูแทนที่ เพื่อให้สเปกตรัมการคายแสงเรดชิฟท์ และทำให้โมเลกุลมีสโตรกชิพมากขึ้นซึ่งเหมาะสมแก่การประยุกต์ใช้สี่ข้อมเหล่านี้ในเซลล์สิ่งมีชีวิต

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STATEMENTS OF ORIGINALITY

1. Design the new molecular structure of fluorescent dyes by using computer chemistry, which environmental friendly, save time and this research are the guidance for chemists.
2. Photophysical and photochemical studies of fluorescent dyes. Theoretical studies of heteroatom and substituent effect resulting in the red-shifted emission spectra and large Stokes' shift, which can be applied for biological system.



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