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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
ωB97XD	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
$kcal \cdot mol^{-1}$	Kilocalorie per mole
eV	Electron volts
ICT	Intramolecular charge transfer
PECs	Potential Energy Curves

APBT	2-(2′-Aminophenyl)benzothiazole
AzPBT	2-(2′-Azidophenyl)benzothiazole

LIST OF SYMBOLS

S	Excited singlet state
T	Excited triplet state
υ	Frequency
S_0	Ground state
S_1	First excited singlet state
S_2	Second excited singlet state
T_1	First excited triplet state
°	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-obital
$\hat{f}$	Fock operator
ε_i	Spin-obital 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
ππ* and π-π*	Pi to pi* transition (proton transfer)
nπ* and n-π*	n to Pi* transition (intramolecular charge transfer)
Å	Angstrom
ΔE	Relative energy
%	Percent
f	Oscillator strength
Δλ	Deviation between the calculated and experimental wavelength

ข้อความแห่งการริเริ่ม

1) การออกแบบโมเลกุลสีย้อมฟลูออเรสเซนต์ตัวใหม่โดยวิธีการทางเคมีคอมพิวเตอร์ซึ่งเป็นมิตรต่อสิ่งแวดล้อม ปราศจากสารเคมีที่เป็นพิษ ประหยัดเวลาและเป็นแนวทางสำคัญในกระบวนการสังเคราะห์แก่นักเคมี

2) การศึกษาสมบัติแสงเชิงฟิสิกส์และแสงเชิงเคมีของสีย้อมฟลูออเรสเซนต์โดยการเติมเฮเทอโรอะตอมหรือหมู่แทนที่ เพื่อทำให้สเปกตรัมการคายแสงเรดชิฟท์ และทำให้โมเลกุลมีสโตรกชิพมากขึ้นซึ่งเหมาะสมแก่การประยุกต์ใช้สีย้อมเหล่านี้ในเซลล์สิ่งมีชีวิต

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.