Chapter 1

Introductory Chapter: Iridium Complexes as Organic Light Emitting Diodes (OLEDs): A Theoretical Analysis

Ruby Srivastava

Additional information is available at the end of the chapter

http://dx.doi.org/10.5772/intechopen.78398

1. Introduction

A specific discipline of electronics, which focus on light-emitting or light-detecting devices, the term "Optoelectronics" is used in the broader perspective. Such devices include those that emit light (LEDs and light bulbs), channel light (fiber optic cables), detect light (photodiodes and photoresistors), or are controlled by light (optoisolators and phototransistors). An interesting combination of electronics and optics, Optoelectronics find varied applications in telecommunications, military services, medical field, solid state devices (sensors, IR emitters, and laser emitters), and automatic control systems. The other counterparts as photo resistors and photovoltaic devices are also used for various applications. Nowadays, photodetectors has confronted significant challenges regarding the realization of efficient and sensitive detection with low-noise for the ultraviolet (UV), visible, and infrared regimes of electromagnetic spectrum.

Cyclometalated Ir(III) complexes are used as the organic light emitting diode (OLED) phosphors due to the phosphorescent emission, which spans the whole visible spectrum. These complexes are the most effective and tunable phosphorescent material for OLED devices due to their higher internal quantum efficiency compared to the fluorescent ones (3, 1) [1, 2]. These complexes can be used as photocatalysts for CO_2 reduction, catalysts for chemical reactions. Biological reagents and photo-oxidants: Few parameters which can lead to the success of these complexes are emission, color tunability, stability, strong spin-orbit coupling, triplet quantum yield, and efficiency toward the radiative transitions. Studies on the homoleptic and heteroleptic iridium complexes are carried out in the absorption spectrum, which lies in the UV-visible region (**Figure 1**).

The synthesis and photophysics of Ir(III) complexes have been of great interest as OLEDs as these complexes represent the most effective, tunable, and sublimable phosphorescent materials.

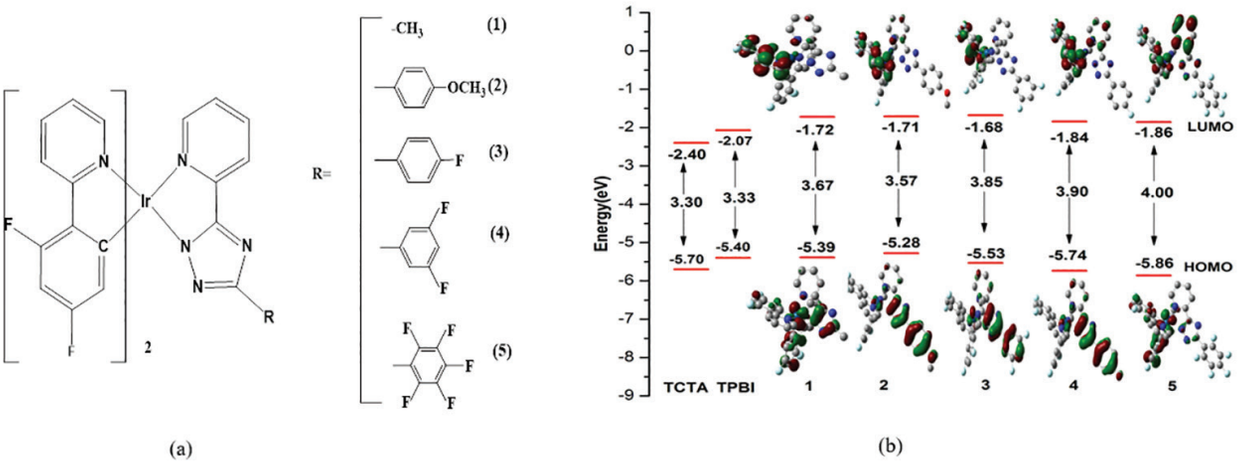

Figure 1. (a) Illustration of five Ir complexes and (b) a pictorial representation of energy highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO) of the given complexes along with the host materials (Tris(4-carbazoyl-9-ylphenyl)amine (TCTA) and 2,2′,2″-1,3,5-Tris(1-phenyl-1H-benzimidazol- 2-yl)benzene (TPBI)).

OLEDs are also utilized as sensors, probes, imaging agents, and photosensitizers for electron and energy transfer. Till now the fabrication of red and green emitting Ir(III) complexes have been successfully fabricated with high-quantum efficiencies, but achieving phosphorescence with high-quantum efficiency for blue light emitting OLEDs is still a challenge. Therefore, several strategies have been developed on how to shift the emission to a blue color. Apart from experimental results theoretical results have been taken to measure the efficiency of blue OLEDs by computational methodologies. Therefore, here we will discuss the theoretical methodology used in design complexes to predict the blue color.

2. Theoretical measurements

The theoretical measures are initialed by the geometrical stability of the electronic structures of these complexes, the nature-type as well as the percentage molecular orbital contributions from the different ligands, absorption spectra in solvent, and the evaluation of excited state lifetimes. Later on, evaluation of the spin-orbital coupling (SOC) matrix element and the predictive measurements are used to calculate the radiative rate constant k_r, and lastly the phosphorescent properties and the better performance of the OLED are discussed, which include the charge injection/transport and balance ability, the energy transfer rate, and triplet exciton confinement for host and guest materials [3]. In some design complexes, two host materials are also suggested for device structure comparing their triplet energies and charge transport properties for the studied guest complexes [4] (**Figure 2**).

The ionization potential (IP), electron affinity (EA), hole extraction potential (HEP), electron extraction potential (EEP), reorganization energy (λ), and HOMO-LUMO gap (HL) HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) are calculated by Gaussian and ADF software. The basis sets and functional are used as per requirements of the design complexes.

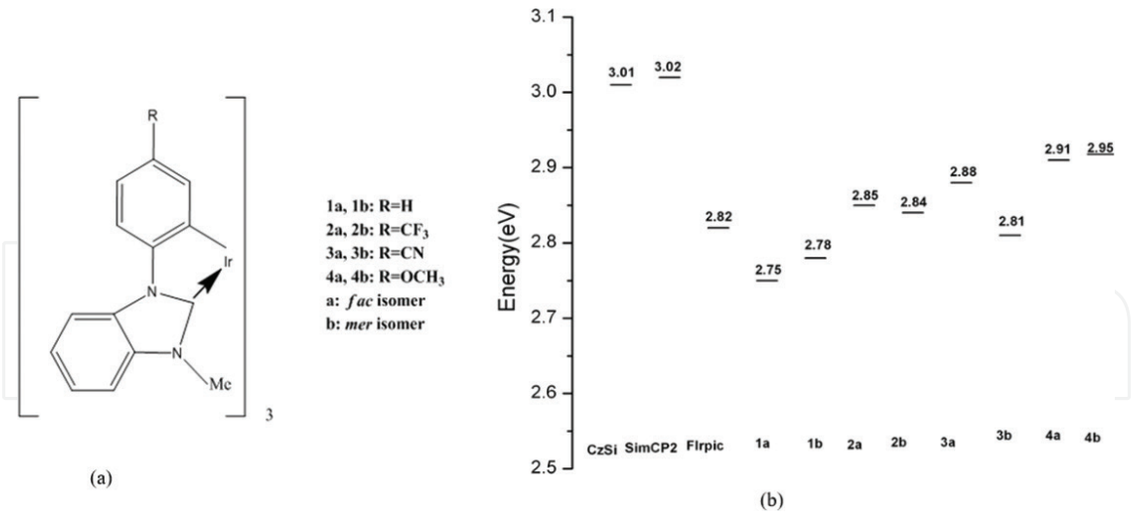

Figure 2. (a) Illustration of eight Ir complexes and (b) triplet energy representation of the eight complexes along with the triplet energy of host materials (CzSi, SimCP2, and FIrpic).

3. Results

The first step is to look into the ground state electronic structures, as the observed differences in the optoelectronic and photophysical properties depend on the electronic structures. Frontier molecular orbital (FMO) also plays a key role in gaining a better understanding of the optical and chemical properties. A detailed examination of the pertinent orbitals is carried out to see the HOMO and LUMO energies. For the singlet-triplet transitions, it is easy to take the first 10 leading excited states (with CI coefficients) and the first triplet energy states. On the basis of the optimized structures in the excited state, the emission spectra of the considered molecules are investigated. The good performance of an OLED device depends on the charge mobilities and a comparable balance between the hole and electron transport, it is necessary to calculate the charge injection properties as ionization potentials (IPs), electron affinities (EAs), HOMO and LUMO, reorganization energy, hole and electron extraction potentials (HEP, EEP). For the photoluminescent materials, it is anticipated that lower the IP of the emitter, the easier the entrance of holes from the hole-transport layer (HTL) to the emitter, and the higher the EA of the emitter, the easier the entrance of electrons from the electron-transport layer (ETL). Solvent polarization energy (SPE) is also used to estimate the self-trapping energies of charge in the materials, which is the energy due to the structural relaxation. The studies of the guest-host relationship are also important as the efficiency of OLEDs is improved on the basis of these investigations. As iridium phosphors have to be widely spread into the host matrix, a relatively long phosphorescence time for metal complexes can cause a long range of exciton diffusion, which may lead to dominant triplet-triplet annihilation. This will get quenched in the adjacent layers of materials in OLEDs. Here it is to mention that an effective host material is very important to achieve efficient electrophosphorescence. Several other requirements for the effective host material are (a) HOMOs and the LUMOs of the host material should match those of neighboring

active layers to lower the device driving voltage and reduce the hole and electron injection barrier. (b) The host should possess higher triplet energies than those of the dopant emitters so as to confine the triplet excitons in the emissive layer and to prevent reverse energy transfer from the guest back to the host. (c) The charge carrier transport properties of the host have to be good and it should balance the hole-electron recombination process. Dexter energy transfer also plays a significant role in obtaining the triplet excitons for the guest materials and the corresponding rate is correlated with the changes in Gibbs free energy (triplet energy difference) based on the Marcus electron-transfer theory.

Thus, we can say that though the OLED development is more of an experimental field than being a theoretically determined science. Nevertheless, the key parameters discussed here can be reliably considered in the theory and this knowledge will surely help in the design and fabrication of new phosphorescent OLEDs.

Acknowledgements

I acknowledge the financial assistance by the DST WOS A project (SR/WOS A/CS-1005/2014). I am also thankful to my Mentor Dr. G. Narahari Sastry, Center for Molecular Modeling, CSIR-Indian Institute of Chemical Technology for the support.

Author details

Ruby Srivastava

Address all correspondence to: amitruby1@gmail.com

CSIR-IICT, Hyderabad, India

References

[1] Srivastava R, Laxmikanth Rao J, Kotamarthi B. Theoretical study of electronic structures and opto-electronic properties of iridium(III) complexes containing benzoxazole derivatives and different ancillary β-diketonate ligands. Computational and Theoretical Chemistry. 2014;**1035**:51-59. DOI: 10.1016/j.comptc.2014.02.026

[2] Srivastava R, Kada Y, Kotamarthi B. Theoretical studies of electronic structures and opto-electronic properties of blue emitting heteroleptic Iridium(III) complexes containing 1,1 dithiolates. Computational and Theoretical Chemistry. 2013;**1009**:35-42. DOI: 10.1016/j.comptc.2012.12.032

[3] Srivastava R, Laxmikanth Rao J. The effect of substituted 1,2,4-triazole moiety on the emission, phosphorescent properties of the blue emitting heteroleptic Iridium(III) complexes and the OLED performance: A theoretical study. Physical Chemistry Chemical Physics. 2014;**16**:17284. DOI: 10.1039/c4cp02368d

[4] Srivastava R. The effect of substituted moiety on the optoelectronic and photophysical properties of tris (phenyl benzimidazolinato) Ir(III) carbene complexes and the OLED performance: A theoretical study. Molecular Physics. 2015;**113**(12):1451-1464. DOI: 10.1080/00268976.2014.1002824

IntechOpen