DOCTORAL THESIS

Synthesis, structures, photophysics and optoelectronic properties of metalated molecular materials derived from multifunctional chromophores

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Synthesis, Structures, Photophysics and Optoelectronic Properties of Metalated Molecular Materials Derived from Multifunctional Chromophores

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Abstract

The molecular design, synthesis, spectroscopic and photophysical characterization of a series of new transition metal-containing complexes and polymers incorporating various functional chromophores are discussed. The roles played by these multifunctional metalated materials in various domains of optoelectronics are presented in terms of their structure-property-function relationships.

Chapter 1 contains a brief overview of the development of molecular and polymeric materials in the fields of organic light-emitting diodes (OLEDs) and solar cells with particular reference to the background theory and the molecular design concepts of various molecular units.

Chapter 2 presents the synthesis, structural, photophysical, electrochemical and electroluminescent properties of a novel class of trifunctional platinum(II) cyclometalated complexes in which the hole-transporting triarylamine, electron-transporting oxadiazole and electroluminescent metal components are integrated into a single molecule. Substituents with different electronic properties were introduced into the bipolar cyclometalating ligands to fine-tune the absorption and emissive characteristics of the compounds and the results were correlated with theoretical calculations using density functional theory. Comparison of the photophysics and electrochemistry of our multifunctional systems to those only derived from each of the constituent components was also

made and discussed. These sublimable complexes can be used for the fabrication of monochromatic electrophosphorescent devices and their utilization in the realization of white light OLEDs is also discussed.

A full account of the preparation, characterization and optical properties of some luminescent group 10–12 transition metal alkynyl complexes that have hole-transporting triarylamine and electron-transporting oxadiazole moieties are described in Chapter 3. We report the photoluminescence and redox properties of these metal acetylide compounds in terms of the ligand substituent effects and the nature of metal groups and the results were correlated with computational data based on the density functional theory. The heavy-metal effects in harnessing the phosphorescence emissions and the observation of solvatochromic behavior in some of these materials were also discussed.

In Chapter 4, novel synthetic strategies were developed to prepare a new structural class of solution-processable and thermally stable metallopolyynes of platinum and mercury functionalized with well-defined fluorene-oxadiazole oligomers. The regiochemical structures of these metallopolymers were studied by NMR and IR spectroscopies. We compare their optical absorption and photoluminescence spectra with their dinuclear model complexes of group 10–12 transition elements.

Chapter 5 outlines the new approaches to the synthesis of some low band gap organometallic polyynes and diynes of platinum based on the donor-acceptor design concept. As a promising step towards our goal in designing metal polyynes

of narrow band gaps, we have exploited the bithiazole-oligothiophene and benzothiadiazole-oligothiophene as the core components to create a new π-conjugated system with extended absorption that features unique donor-acceptor characteristics. These materials absorb strongly in the visible region and possess high solution processability. The potential of using these low band gap polymeric materials in the fabrication of highly efficient polymer solar cells has been examined with good performance characteristics.

Chapters 6 and 7 present the concluding remarks and the experimental details of the work presented in Chapters 2–5.

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