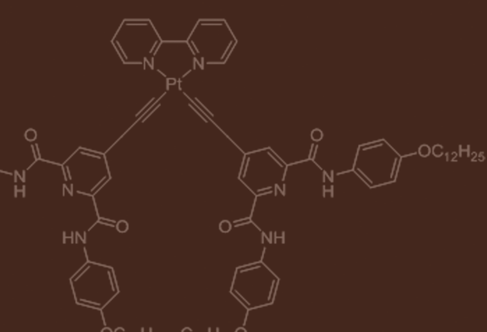
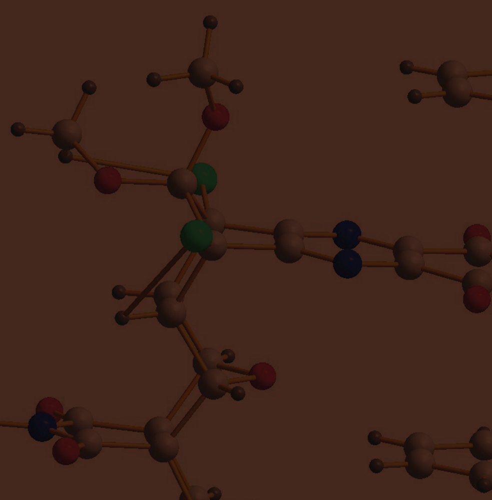
ORGANIC STRUCTURE DESIGN

APPLICATIONS IN OPTICAL AND ELECTRONIC DEVICES

edited by
Tahsin J. Chow





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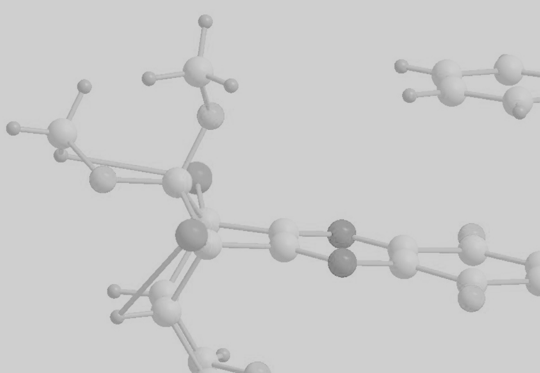

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Contents

Preface

The application of organic materials to optical and electronic devices is a fast-growing research area nowadays. These new type of materials are expected to be the mainstream in the next generation of smart machines. They combine the classical electronic properties of metals, yet with the advantages of organic matters, such as softness, light weight, good solubility, and high structural flexibility. The choice of molecular structures is versatile, such as extended π-conjugate systems and macrocycles with special shapes. The functional properties include light-emitting diodes (OLEDs), organic photovoltaics (OPVs), field-effect transistors (OFETs), artificial machines, and chemical sensors. This book provides a review on several top-notch topics in these areas. The contents are mainly focused on the design and synthesis of organic functional molecules but also include related topics such as the model study on electron transfer phenomena and the fabrication technologies of organic nanostructures.

The key features in this book may be grouped into the following categories: (1) molecular design and synthesis of functional compounds of organic and organometallic molecules in forms discrete and polymeric structures; (2) solution-processed fabrication technologies, nanostructure growth and crystallization, electro-polymerization of organic amines, supramolecular assemblies of organogels; (3) principles of long-range electron transfer through organic media, and for the design of donor–acceptor dipolar compounds; and (4) evaluation of device performance with respect to structural designs, for the application to light-emitting diodes, organic solar cells, field-effect transistors, artificial machines, and chemical sensors. The following gives a brief outline of each chapter.

To make a single molecule work as a functional device, several active sites have to be implanted onto a common molecular backbone so that they can communicate effectively in a designated manner. In these systems, electron and/or energy transfer processes are involved. In order to control the flow of electron/energy, the mechanism of electronic coupling must be realized. The construction of theoretical models by using computational methods is reviewed in Chapter 1.

An overall view on organic nano- and micro materials constructed by the solution process and their applications is described in Chapter 2. The design strategies, various growth mechanisms, and device performances of OFETs, OLEDs, OPVs, photo-detectors, and super-hydrophobic materials are summarized. In comparison with physical vapor deposition, solution processing provides a more convenient and cost-effective approach to obtain organic nano- and micro materials with various morphologies, including wires, sheets, and flowers. Their relationships with the corresponding applications are discussed based on the general concepts of supramolecular chemistry.

The π–π interaction in organic molecules plays a fundamental role in many processes, such as the self-assembly for supramolecular stacking, light-harvesting antennae for photosynthesis, amyloid fibril formation in a variety of diseases, double-helix structure of DNA, and so on. The study of electron/energy transfer processes in organic structures depends on the understanding of their π–π interactions. In Chapter 3, the electron movement in π-stacked linear arrays, namely the multilayered [3.3]paracyclophanes, is examined by their transient absorption spectra of radical cation species. Their electron/charge transfer mechanism is regarded as analogous to that of the double strand DNA molecules.

One of the ultimate goals in the development of functional molecules is to assemble an artificial machine at the molecular level. The mechanical work of ATP synthase involves the rotation of a central stalk that is powered by electrochemical potential energy created by the concentration gradient of proton across the inner membrane of mitochondria. As inspired by ATP synthase and other biological molecular machines, the development of artificial molecular machines has been an important subject of nanoscience and nanotechnology. Chapter 4 reviews the progress of molecular design and functions of molecular machines, with a special emphasis on molecular rotors. The rotation of the rotors is gated by light and/or electrical energy as energy sources.

The principle and efficiency of the related photochemistry and electrochemistry are discussed.

Supramolecular gels are semisolid materials, which can serve a variety of purposes and appear ubiquitously in our daily lives in a variety of forms. Gels are prevalent in nature, within cells and tissues of bodies, and are also present in a variety of artificial materials, including toothpaste, soap, shampoo, hair gel, contact lenses, and gel pens. These materials self-assemble through the formation of non-covalent intermolecular interactions to form supramolecular networks that trap solvent within their matrices. Because of the non-covalent nature of the forces of self-assembly, the gelation process is typically thermally reversible. In Chapter 5, various types of organogelators, mainly including those grafted with amide functionalities, are reviewed.

The pharmacological importance of quinoxalines and their utility as building blocks for preparing organic electronic materials have motivated a considerable number of studies in recent years. The synthetic approaches to multi-bridged U, N, and Z-shaped artificial compounds embedded with quinoxaline units are described in Chapter 6. The synthesis was executed efficiently mainly by three fundamental reactions, i.e., Diels–Alder reaction, oxidation with RuO_4, and carbonyl-amine condensation reaction. These compounds may possess specific functions of interest, such as electron/energy transfer phenomena, host–guest complexation, and pharmaceutical applications.

Calixarenes are $[1_n]$ metacyclophanes, which are derived from the condensation of phenols and formaldehyde in different conditions. Gutsche coined the term “calix[4]arenes,” which is derived from Latin “calyx,” which means vase, pointing out the presence of a cup-shape structure in these macrocycles when they assume the *cone* conformation, where all four aryl groups are oriented to the same direction. In Chapter 7, a series of calix[4]arene derivatives containing various bifunctional groups were prepared by using “click chemistry,” where metal ions can be encircled making them useful fluorescent sensors.

The contents of Chapter 8 are focused on the electron-transporting materials (ETMs) of OLEDs. The major objective is to glean a variety of structure types from a comprehensive survey of organic compounds that are exploited for application as ETMs and identify key structural elements/motifs that allow design and development of newer materials with improved device performances. Although limited to ETMs, the insights that are developed in this chapter will apply equally to all other types of materials, viz., hole-transporting materials, emissive materials, etc., that are relevant to OLED device constructions.

To fabricate thin-film organic electronic devices, polymeric materials are usually coated as uniform thin films directly on an electrode by spin casting. It requires good solubility of the polymers in an appropriate solvent. The low solubility of conjugated polymers limits their use on optoelectronic applications. Direct film formation on ITO glass by electro-polymerization provides an option to bypass the solubility problem. In Chapter 9, some fundamental properties about the chemical reactivity of carbazole and triphenylamine derivatives toward electro-polymerization are reviewed.

Acenes exhibit a strong tendency to form highly ordered films in various substrates under different growth conditions. They can display a high charge mobility in an electric field and, therefore, are recognized as promising materials for the application on OFETs. However, the low solubility of pentacene in most solvents is a major drawback that limited its utility through solution processes. Many efforts have been attempted to prepare "soluble" pentacene precursors in order to go around this problem. In Chapters 10 and 11, new methods for the preparation of acenes are summarized. Workable synthetic schemes are outlined, and can be used as practical guide for the preparation of similar poly-aromatic materials.

The authorship of this book includes eleven renowned professors in the top-rated universities and institutions in Asia: Kyushu University (Teruo Shinmyozu), Peking University (Jian Pei), IIT Kanpur (J. N. Moorthy), National Taiwan University (Jye-Shane Yang and Man-kit Leung), National Chiao Tung University (Wen-Sheng Chung), National Chung Cheng University (Teh-Chang Chou), and Academia Sinica (Chao-Ping Hsu, Shih-Sheng Sun, Chih-Hsiu Lin, and Tahsin J. Chow). Many of the authors have developed long-term research collaboration among themselves. They have made significant efforts to summarize their best results and integrated into the contents of this book. It provides the first-hand reference information to the readers who are interested in the progresses of the emerging new field of organic optoelectronic materials.