EMERGING MATERIALS AND TECHNOLOGIES

Computational Studies

From Molecules to Materials

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Contents

11 Organic Semiconducting Materials in Electronic Devices

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11.1 INTRODUCTION

Organic semiconductors are widely utilized now as alternative silicon-based inorganic semiconducting materials in electronic devices. The 2000's Nobel Prize in chemistry was given to Alan Heeger, Alan MacDiarmid, and Hideki Shirakawa for the discovery and development of conductive polymer. Their experiments conducted in 1970–1980 with trans-polyacetylene showed that it was possible to determine the conductivity of covalent organic material by exposing it to vapors of chlorine, bromine, or iodine.[1] Also in the 1960s, Weiss and coworkers already demonstrated electrical conductivity in iodine-doped oxidized polypyrrole, and in 1965 electroluminescence was observed in anthracene crystals by Kallmann et al.,[2] Today, interest in organic electronics is increased due to the demand for alternating substitutes of Si-based electronics or inorganic materials-based electronics that could offer easier synthesis and processability.[3] One of the key differences between inorganic and organic semiconductors lies in their processing techniques. Inorganic semiconductors are processed through an expensive technique that requires highly pure-quality crystalline substrates. Organic semiconductors don't need such processing techniques, and they can be deposited over inexpensive substrates such as glass, plastic, etc.[4] Synthesis techniques for organics are readily available like spin-coating, drop-casting, and direct printing via stamps or inkjets. Their compatibility with lightweight, mechanically flexible plastic substrates and innovative fabrication routes makes them possible candidates for future electronic devices. Moreover, due to different molecular tailoring possibilities via chemical synthesis, organic materials present a wide variety in functionality.[5] The design of the molecular structures can be engineered to enhance properties like band gap modification of the materials. Modification of the chemical end groups also allows the fabrication of large transistor arrays for organic sensors.[6] Different methods are developed to increase the sensitivity and selectivity of organic sensing transistors to different chemical or biological species. There has been a rapid progress in the industrial development of organic electronic devices. Organic devices are suitable for large-scale application areas where their operation can offer high performance, reliability, stability, long lifetime, good control, and reproducibility.[7] As a constituent of plastic electronic components, organic semiconductors have arrived at a good place.

Organic materials can be divided broadly into two categories: small molecules and polymers.[8] *Small molecules* are the simplest type of organic solids, and, despite their small size, they can be relatively massive, with typical masses of several hundred atomic mass units (amu). Regardless of their size, all small molecules are distinct units with identical structures. *Polymers* are the long chains of repeating units based on a backbone of carbon-containing bonds. Polymer masses are very large, and their masses vary from tens to thousands of repeating units up to a million amu. The complexity of semiconducting polymers also varies greatly, from relatively simple polythiophenes to intricate donor–acceptor complexes.[9]

Charge transport within organic materials is a combination of two processes: intramolecular carrier movement and intermolecular charge transfer. In the organic molecular complexes, π-bond conjugation helps in charge carriers to move freely but, due to the weak van der Waal forces, the charge transport is limited, and it lowers charge carrier mobility to typical values of 10^{-5} to 10^{-2} $cm^2\ V^{-1}\ s^{-1}$ in organic photovoltaics.[10]

Charge carriers are strongly localized on individual molecules, and the intermolecular transport occurs through a hopping process as a charge carrier overcomes an energy barrier to move from

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