

Lecture Notes in Electrical Engineering 1370

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Emerging Technologies with Advanced Devices from Micro to Nano

ETMN 2024

MOREMEDIA



Springer

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ISSN 1876-1100

ISSN 1876-1119 (electronic)

Lecture Notes in Electrical Engineering

ISBN 978-3-031-84330-3

ISBN 978-3-031-84331-0 (eBook)

<https://doi.org/10.1007/978-3-031-84331-0>

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Contents

| | |
|---|----|
| A Refractive Index-Based Plasmonic Sensor with Enhanced Figure of Merit Using Titanate Material in a Three-Layer Heterostructure | 1 |
| R. Runthala, K. Srivastava, A. Shetty, and P. Arora | |
| Custard Apple Peel Biochar-Based Nanocomposite as a Novel Adsorbent for Removal of Acid Red 114 Dye: Adsorption and Phytotoxicity Studies | 11 |
| Shivanshi Tyagi, Riti Thapar Kapoor, and Rachana Singh | |
| Sustainable Fabrication of Palladium Nanoparticles Coated Cotton Fabric Using <i>Citrus limon</i> Leaf Extract | 21 |
| Savy Panamkuttiyiel Minal and Soam Prakash | |
| Fabrication and Characterization of a Film Bulk Acoustic Wave Resonator Using ZnO Piezo-Layer | 29 |
| Sk. Masiul Islam, Hemant Saini, Vinita, and Jitendra Singh | |
| The Atomically Thin Few-Layer of WS₂ Nanosheets in the Field Effect Transistor Application | 35 |
| Arpita Roy and Biplob Mondal | |
| Influence of Hydroxyapatite Content on the Wear Behavior of Mg-Sn Composites | 43 |
| Sandeep Kumar Jhamb, Ashish Goyal, and Anand Pandey | |
| Coating of Au-Pd Bimetallic Nanoparticles on Cotton Fabric | 53 |
| Savy Panamkuttiyiel Minal and Soam Prakash | |
| Modelling of n-type Materials Based on [D-π-A] Structure for the Application in Organic Field Effect Transistors: DFT Study | 63 |
| Ankit Kargeti, Tabish Rasheed, and Shamoon Ahmad Siddiqui | |

Modelling of n-type Materials Based on [D- π -A] Structure for the Application in Organic Field Effect Transistors: DFT Study



Ankit Kargeti, Tabish Rasheed, and Shamooun Ahmad Siddiqui

Abstract OFETs (Organic Field Effect Transistors) are widely researched since the first reported OFET in 1986 which was made of Polythiophene. We designed two novel molecular structures based on Donor- π -Acceptor or [D- π -A] model to look upon their efficient use in Organic field effect transistors. The designed systems are named as system first S1 (anthracene-pyrrole-butanoic acid), and system second S2 (naphthalene-pyrrole-butanoic acid). Both the structures were optimized under the framework of density functional theory with B3LYP/6-31 + G(d, p) basis set on a Gaussian16W software package. The calculated parameters are hole's reorganization energy λ_h , electron's reorganization energy λ_e , HOMO-LUMO energy gap, dipole moment. Further, we have looked upon their electric field dependence of the HOMO-LUMO energy gap and dipole moment for all the molecules. Both the designed molecules S1 and S2, are found to be suitable for designing as n-type semiconducting channel for OFETs.

Keywords OFET · D- π -A · n-Type and p-Type semiconductors · DFT · HOMO-LUMO gap energy · Reorganization energy of holes and electrons

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