

Accepted Manuscript

Title: Tuning of optoelectronic and charge transport properties in star shaped anthracenothiophene-pyrimidine derivatives as multifunctional materials

Authors: Ahmad Irfan, Shabbir Muhammad, Aijaz Rasool Chaudhry, Abdullah G. Al-Sehemi, Ruifa Jin



PII: S0030-4026(17)31126-9
DOI: <http://dx.doi.org/10.1016/j.ijleo.2017.09.065>
Reference: IJLEO 59673

To appear in:

Received date: 2-6-2017
Accepted date: 18-9-2017

Please cite this article as: Ahmad Irfan, Shabbir Muhammad, Aijaz Rasool Chaudhry, Abdullah G. Al-Sehemi, Ruifa Jin, Tuning of optoelectronic and charge transport properties in star shaped anthracenothiophene-pyrimidine derivatives as multifunctional materials, *Optik - International Journal for Light and Electron Optics* <http://dx.doi.org/10.1016/j.ijleo.2017.09.065>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Tuning of optoelectronic and charge transport properties in star shaped anthracenothiophene-pyrimidine derivatives as multifunctional materials

Ahmad Irfan^{a,b*}, Shabbir Muhammad^{a,c}, Aijaz Rasool Chaudhry^{a,c}, Abdullah G. Al-Sehemi^{a,b}, Ruifa Jin^d

^a Department of Chemistry, Faculty of Science, King Khalid University, Abha 61413, P.O. Box 9004, Saudi Arabia

^b Research Center for Advanced Materials Science (RCAMS), King Khalid University, Abha 61413, P.O. Box 9004, Saudi Arabia

^c Department of Physics, Faculty of Science, King Khalid University, Abha 61413, P.O. Box 9004, Saudi Arabia

^d College of Chemistry and Chemical Engineering, Chifeng University, Chifeng 024000, China

Abstract

With the aim to tune the optoelectronic, charge transport and nonlinear optical properties, four novel star shaped compounds were designed from the initial structure 4,6-di-(anthracenothiophen-2-yl)pyrimidine (DATP). The (2,5-di-(thiophen-2-yl)-4,6-di-(anthracenothiophen-2-yl)pyrimidine) (**1**), (2,5-di(benzo-thiophen-2-yl)-4,6-di-(anthracenothiophen-2-yl)pyrimidine) (**2**), 2,5-di(naphthothiophen-2-yl)-4,6-di-(anthracene-thiophen-2-yl)-pyrimidine (**3**), and 2,4,5,6-tetrakis(anthracene-thiophen-2-yl)pyrimidine (**4**) were deliberated by substituting the thiophene, benzothiophene, naphthothiophene and anthracenothiophene moieties at positions 2 and 5 of the pyrimidine unit in DATP, respectively. The ground and excited state geometries were optimized by adopting the density functional theory (DFT) and time-dependent DFT at B3LYP/6-31G** and TD-B3LYP/6-31G** level of theories, respectively. We shed light on the energies of the frontier molecular orbitals (FMOs), energy gaps (E_{gaps}), absorption, fluorescence, total/partial density of

* Corresponding author: Ahmad Irfan
E-mail: irfaahmad@gmail.com
Tel.:00966172419481
Fax:00966172418426

Download English Version:

<https://daneshyari.com/en/article/5025116>

Download Persian Version:

<https://daneshyari.com/article/5025116>

[Daneshyari.com](https://daneshyari.com)