Computational and Theoretical Chemistry 977 (2011) 9–12

Contents lists available at SciVerse ScienceDirect

Computational and Theoretical Chemistry

journal homepage: www.elsevier.com/locate/comptc

A study on the electronic and charge transfer properties in tin phthalocyanine (SnPc) derivatives by density functional theory

Ahmad Irfan [a,*,1], Abdullah G. Al-Sehemi [a,*], Abdullah M. Asiri [b,c], Muhammad Nadeem [d,2], Khalid A. Alamry [b]

[a] Chemistry Department, Faculty of Science, King Khalid University, Abha, Saudi Arabia
[b] Chemistry Department, Faculty of Science, King Abdulaziz University, P.O. Box 80203, Jeddah 21589, Saudi Arabia
[c] The Center of Excellence for Advance Materials Research, King Abdulaziz University, P.O. Box 80203, Jeddah 21589, Saudi Arabia
[d] Department of Chemistry, University of Agriculture, Faisalabad 38040, Punjab, Pakistan

ARTICLE INFO

Article history:
Received 20 June 2011
Received in revised form 27 August 2011
Accepted 28 August 2011
Available online 10 September 2011

Keywords:
Optical materials
HOMO
LUMO
Optical properties
Reorganization energy

ABSTRACT

The carrier transport properties of tin phthalocyanine (SnPc) derivatives have been investigated at DFT/B3LYP/(6-31G*, LANL2DZ) level. Contributions from the Boron and Nitrogen atoms are found to be predominant in the HOMOs. Moreover, the systems SnPcBN3, SnPcBN4 and SnPcBN5 have lower LUMO energy in comparison to SnPc. Introduction of BH (at position 1, 2 and 3) and NH (at position 4) onto the SnPc molecule induces the increase in both the vertical ionization potential (IPv) and vertical electronic affinity (EAv) for SnPcBN3, SnPcBN4, SnPcBN5 versus SnPc. These results indicate the increased injection barrier for hole and decreased injection barrier for electron transfer. On the other hand, both IPv and EAv for SnPcBN1, SnPcBN2 are decreased to SnPc revealing the decreased and increased injection barrier for hole and electron transport, respectively. It has been predicted that SnPcBN3, SnPcBN4, SnPcBN5 would be better electron transfer materials while SnPcBN1, SnPcBN2 behave as better hole transporter.

1. Introduction

Organic devices, such as photovoltaic cells (OPVs) and field-effect transistors (OFETs), produced by solution processes own certain advantages such as large area, flexibility, lower temperatures and cost effective route for the device fabrication. In general, organic semiconductors are known to possess small carrier mobility compared to inorganic ones, because of the molecular nature of organic materials. Recently, the performance of organic devices has been improved [1–3]. Some small molecular compounds with a large π-conjugated ring structure, such as phthalocyanines, pentacene, rubrene, and porphyrins have been demonstrated as good semiconductors [4–7]. Many organic semiconductors reported so far are unipolar and exhibit p-type transport properties, whereas more efforts have been devoted to the design and synthesis of n-channel materials in recent years. Few organic semiconductors have been found to exhibit ambipolar properties [8]. Moreover, very few organic semiconductors exhibit balanced hole and electron transport characteristics [9–11].

Ambipolar materials are strongly desirable for logic circuit design because they enable the simple fabrication of complementary circuits like inverters without advanced patterning techniques to deposit p- and n-channel materials separately. Moreover, ambipolar materials work for both positive and negative voltages which streamlines the circuit design. An ideal ambipolar material is expected to give balanced performance in both negative and positive voltage regimes; therefore, it is strongly desired that the ambipolar materials should possess balanced n- and p-channel performance.

Phthalocyanines have gained attention in OFETs for many years because of their remarkably high chemical and thermal stabilities, as well as non-toxicity and better field-effect properties [12,13]. The unique properties of phthalocyanine dyes and pigments enables them to be the colorant of choice for most blue and green colors. Phthalocyanines are also finding extensive use in modern hi-tech areas [14].

The tin phthalocyanine (SnPc) is typical phthalocyanine using in OFETs [15,16]. Previous quantum chemical studies revealed that boron-substituted hetroacene is good to design electron transport and ambipolar materials while the nitrogen-substituted hetroacene revealed improved hole injection [17–19]. Thus five SnPc

* Corresponding authors.
E-mail addresses: irfaahmad@gmail.com (A. Irfan), agmasq@gmail.com (A.G. Al-Sehemi).
[1] Previously at: Institute of Chemistry, University of the Punjab, Lahore 54590, Pakistan.
[2] Present address: Subsurface Technology, Petronas Research Sdn Bhd. (PRSB), Bangi 43300, Selangor, Malaysia.

2210-271X/$ - see front matter © 2011 Elsevier B.V. All rights reserved.
doi:10.1016/j.comptc.2011.08.030