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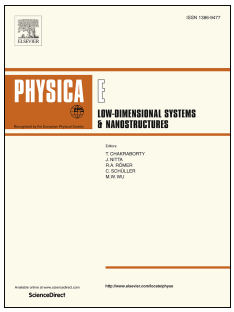

Large thermoelectric efficiency of doped polythiophene junction: A density functional study

Zahra Golsanamlou, Meysam Bagheri Tagani, Hamid Rahimpour Soleimani

PII: S1386-9477(18)30038-9

DOI: 10.1016/j.physe.2018.02.024

Reference: PHYSE 13063

To appear in: *Physica E: Low-dimensional Systems and Nanostructures*

Received Date: 10 January 2018

Revised Date: 6 February 2018

Accepted Date: 22 February 2018

Please cite this article as: Z. Golsanamlou, M. Bagheri Tagani, H. Rahimpour Soleimani, Large thermoelectric efficiency of doped polythiophene junction: A density functional study, *Physica E: Low-dimensional Systems and Nanostructures* (2018), doi: 10.1016/j.physe.2018.02.024.

Large thermoelectric efficiency of doped polythiophene junction: a density functional study

Zahra Golsanamlou, Meysam Bagheri Tagani[1], Hamid Rahimpour Soleimani

Address: Department of Physics, Computational Nanophysics Laboratory (CNL), University of Guilan, Po Box:41335-1914, Rasht, Iran.

Abstract

The thermoelectric properties of polythiophene (PT) coupled to the Au (111) electrodes are studied based on density functional theory with nonequilibrium Green function formalism. Specially, the effect of Li and Cl adsorbents on the thermoelectric efficiency of the PT junction is investigated in different concentrations of the dopants for two lengths of the PT. Results show that the presence of dopants can bring

the structural changes in the oligomer and modify the arrangement of the molecular levels leading to the dramatic changes in the transmission spectra of the junction. Therefore, the large enhancement in thermopower and consequently figure of merit is obtained by dopants which makes the doped PT junction as a beneficial thermoelectric device.

Keywords: Density functional theory, Polythiophene, n- and p-dopants, Thermoelectric efficiency.

1- Introduction:

p-conjugated molecules are one of the most interesting candidates for low cost electronics like photonic, spintronic and thermoelectric devices [1–7] because of their outstanding properties such as discrete energy levels, Coulomb correlations and interference effects [8–11]. In addition, the properties of the molecules can be controlled through the doping [12–15]. Due to the extensive use of molecular devices based on p-conjugated molecules, the study of the thermoelectric properties of these devices has attracted many attentions [16–18]. The thermoelectric efficiency is the ability of the system to convert the

[1] m_bagheri@guilan.ac.ir