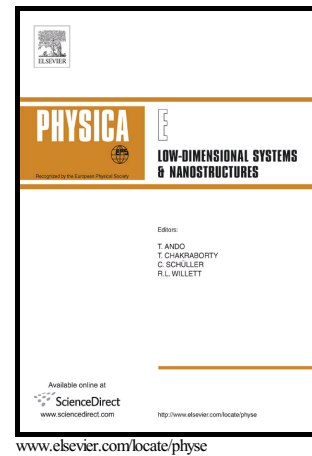


# Author's Accepted Manuscript

Electronic properties of a molecular system with Platinum

J.H. Ojeda, F.G. Medina, David Becerra-Alonso



PII: S1386-9477(17)30718-X  
DOI: <http://dx.doi.org/10.1016/j.physe.2017.07.025>  
Reference: PHYSE12879

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

Received date: 18 May 2017  
Revised date: 25 July 2017  
Accepted date: 27 July 2017

Cite this article as: J.H. Ojeda, F.G. Medina and David Becerra-Alonso  
Electronic properties of a molecular system with Platinum, *Physica E: Low dimensional Systems and Nanostructures*  
<http://dx.doi.org/10.1016/j.physe.2017.07.025>

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 a review of the resulting galley proof before it is published in its final citable 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

# Electronic properties of a molecular system with Platinum

J. H. Ojeda<sup>a,b</sup>, F.G. Medina<sup>a</sup>, David Becerra-Alonso<sup>c</sup>

<sup>a</sup>*Grupo de Física de Materiales, Facultad de Ciencias, Universidad Pedagógica y Tecnológica de Colombia, Tunja, Boyacá, Colombia*

<sup>b</sup>*Laboratorio de Química Teórica y Computacional, Grupo de Investigación Química-Física Molecular y Modelamiento Computacional (QUIMOL), Facultad de Ciencias, Universidad Pedagógica y Tecnológica de Colombia, Tunja, Boyacá, Colombia*

<sup>c</sup>*Department of Quantitative Methods, Universidad Loyola Andalucía-España*

---

## Abstract

The electronic properties are studied using a finite homogeneous molecule called Trans-platinum-linked oligo(tetraethylenes). This system is composed of individual molecules such as benzene rings, platinum, Phosphore and Sulfur. The mechanism for the study of the electron transport through this system is based on placing the molecule between metal contacts to control the current through the molecular system.

We study this molecule based on the tight-binding approach for the calculation of the transport properties using the Landauer-Büttiker formalism and the Fischer-Lee relationship, based on a semi-analytic Green's function method within a real-space renormalization approach. Our results show a significant agreement with experimental measurements.

*Keywords:* Electronic properties, Green's Functions, Renormalization process.

---

## 1. Introduction

Molecular electronics in recent years has been focused on the use of individual atoms or molecules for the construction of electronic circuits. This has generated a reduction on the size of these devices and thus prompted a high interest in the analysis of the effectiveness of electronic properties. In such devices the atoms or molecules are spatially confined. Interactions can arise from electron-electron, electron-phonon, ion-ion, among others, and can relate to the hopping between electronic orbitals [1–8].

This can play an important role in building new nanoelectronic devices designed to be used as molecular electronic transistors, quantum wires, rectifiers, switches, or storage devices, just to mention a few [9–12]. These devices are characterized by electron transfer, probability of transmis-

sion, I-V characteristic curves, shot noise, thermal transport, negative differential resistance, tunnel magnetoresistance, spin-polarized current, among other properties. These have been studied both experimentally and theoretically [9, 13–17].

Within this framework, we study the electric properties in a molecular-wire-like system or finite homogeneous molecule called *Trans-platinum-linked oligo(tetraethylenes)* (hereafter named as TPtL-molecule), which is composed of individual molecules with a special configuration of benzene rings, platinum, Phosphorus and Sulfur.

This structure has attracted interest due to the implementation in a new nano-electronic device designed to be employed as molecular electronic device.

However, there are few studies on electronic transport through molecular systems that are linked to two electrodes in addition to having a

---

\*judith.ojeda@uptc.edu.co

Download English Version:

<https://daneshyari.com/en/article/5450081>

Download Persian Version:

<https://daneshyari.com/article/5450081>

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