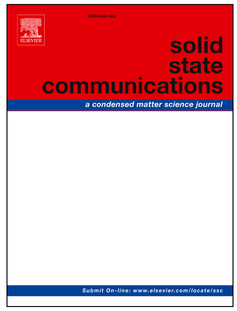

Analytical formula for calculating transmission coefficient of one-dimensional molecules with single impurity

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Analytical formula for calculating transmission coefficient of one-dimensional molecules with single impurity

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Abstract

We have derived a new analytical formula to calculate the transmission coefficient of one-dimensional molecular wires with a single impurity in a convenient and practical way. Such desirable properties can be instantly noticed in the detailed number of adjustable parameters and in the adequately flexible controlling of the chosen position of the impurity in the wire. Furthermore, it is elegantly simple, readily programmable, and reliable. This reasonable conclusion is gained by carefully testing the formula on a considerable number of structures ranging from very simple and basic units and ending with large and complicated systems. As a result, an impressive matching has been found between our analytical model and numerical and analytical calculations of other academic researchers. Such practical comparison supports its undeniable success and reasonable efficiency.

1. Introduction

The advent of molecular devices era has encouraged scientists to seriously and intensively probe its potential features. For instance, they have fabricated unprecedented types of molecules [4, 5], harnessed already existed molecules to perform new tasks [6], innovated new theories to analyze results [7, 8], and derived noval analytical formulae for molecular systems [3, 9-14]. Among these nanoscale systems, conducting molecular chains represent basic but prominent candidates for future nanoelectronics [15-18]. For instance, a highly conductive poly (3,4-ethylenedioxythiophene) poly(styrenesulfonate) (PEDOT:PSS) [19, 20] has been successfully reported to boost the electroluminescence of the molecular device [21], and also gain energy in thermoelectric devices and solar cells[22]. Another example is polyporphyrin oligomers, which shows a mutual relation between its negative differential resistance and junction shape[23]. Such a property would redefine the fabrication rules of molecular junctions, since it determines the conductance of the wire. Moreover, the conductance of a junction that is composed of polyacetylene (PA) attached to graphene (GR) shows the vivid role that a simple pi-conjugated one-dimensional polymer can play in future electronics. The study of Saraiva-Souza *et al.* [24] shows that PA may alter the conductance of the graphene depending on the connection position [24]. These examples and more [25-31], range from sophisticated molecules to simple molecules, shows the variety of structures and implementations of homogeneous one-dimensional molecules. Therefore, understanding such type of molecules is of a particular importance.

The aim of this work is to capture the fingerprints of polymers through an analytical formula. Our mathematical formula is essentially derived to explain the nature of electronic transmission of chain type molecules with a single impurity. Furthermore, the molecules are envisaged via