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First principle study of Lithium impurity effect on energy gap of trans-polyacetylene chain

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Abstract

In this work we have calculated the electronic states of the trans-polyacetylene (t-PA) molecule within the framework of Density Functional Theory (DFT). For this purpose we have used SIESTA code based on the DFT within the Local Density Approximation (LDA). Fully self-consistent Kohn-Sham functional was performed. We used the Ceperley-Alder (CA) form of the exchange-correlation Potential in LDA. Following the above procedures we have calculated Density of State (DOS) of doped t-PA chain. Our results show that, as expected, the energy gap has a considerable decrease with doping.

Keywords: trans-Polyacetylene, Density Functional Theory, Density Of State, Pseudopotential.

Introduction

Recently conductive polymers have received a great interest due to their potential applications for Nano-electronic devices [1]. Their applications in new technology have attracted much attention from both physicists and chemist's society. One of the most interesting polymer materials with huge interest in theoretical and experimental scientific society is t-PA. From the experimental point of view, Polyacetylene has been used in new semiconductor devices [2]. On the other hand, doping it with elements like Lithium, increase it conduction and make it an excellent organic conductor, comparable to metals which can be used in electronic devices.

We have used a linear scaling, fully self-consistent density functional method for performing first-principles calculations, as implemented in SIESTA code [3-5]. In our calculations we have used Density Functional Theory (DFT) based on the work by Hohenberg and Kohn [6] and by Kohn and Sham [7].We have also used the Local Density Approximation (LDA) for the exchange-correlation potential. We used the Ceperley-Alder (CA) form of the exchange-correlation potential in LDA. Troullier-Martins pseudopotentials were used to represent the nuclei plus core electrons [8-9]. In this study, we have calculated DOS and band gap energy of a long t-PA chain and Li doped t-PA which has been discussed in the following section.

Result and discussions

We constructed a unit cell consisting of 8 Carbon and 8 Hydrogen atoms which has been shown in Fig. 1. The distances between C-C, C=C and C-H atoms was selected from experimental data to be 1.429, 1.368 and 1.091 Angstrom, respectively [10].

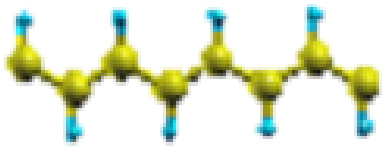
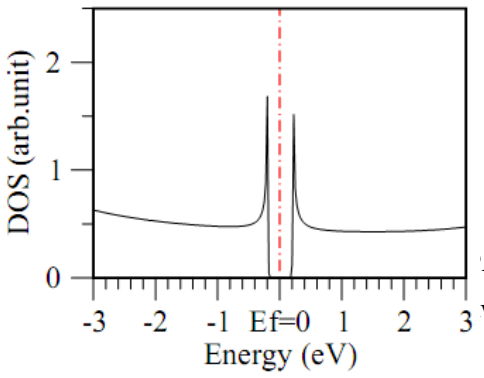


Fig. 1: a diagram of 1D t-PA chain. The yellows are C and blue ones are H atoms. The alternating single and double bonds has not been shown.

Density of State for the 1D t-PA chain has been shown in Fig. 2. The difference between HOMO and LUMO levels around the Fermi energy, which is called energy band gap, was calculated to be 0.4 eV which is comparable to its experimental value.



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We carried on the calculation with doping a Lithium atom in the way that showed in Fig. 3.

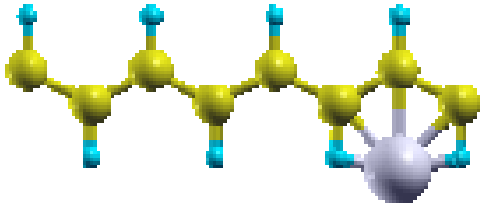

Fig. 3: The geometry of our system. The same as the Fig. 2 but the white shows Li atom.

The Density of State of this system has been shown in Fig. 4. As seems, it's energy gap decrease obviously.

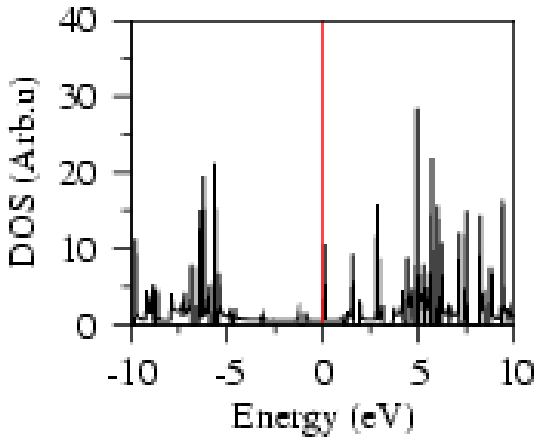

Fig. 4: DOS for the doped t-PA chain.

Since the properties of materials is related to the value of their E_g, it should be possible to control the electronic properties of t-PA in electronic devices and therefore the doped trans-polyacetylene could be a proper candidate in this field.

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