Quasiperiodic CH₂/SiH₂ Molecular Nanowires

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Introduction

Nanotechnology is a fast growing researcher field [1]. With their application, it promises a new industrial revolution, giving us the understanding, production, control, and use of structured matter at the atomic and molecular level, i. e., objects with dimensions from 1 to 100 nanometers, where the physics laws that govern this world is quantum mechanics. Thus, the study of quantum mechanics applied to these miniature systems enables us to discover new and revolutionary directions in science, and the development of new technologies associated with this miniature world, called nanotechnology. Various scientific groups are keen about this technology and are devoting themselves to the development of more, new, and better nanomaterials [2, 3, 4]. In the next decade, the expectation is that no field will be left untouched by the incredible benefits available through application of nanotechnology. Between these news developments, we detach the one-dimensional nanowire [5, 6, 7, 8]. The complete understanding of these nanowires is one important key to further applications in nanotechnology.

In this paper we address to theoretical calculations of the electronic spectra of molecular nanowire where its molecular components are arranged in a Fibonacci quasiperiodic sequence. This nanowire is formed by CH_2 , and SiH_2 radicals. We have used molecular mechanics with universal force field(UFF) for obtain the optimized relaxed structures, and semi-empirical quantum method based on Hückel extended model to obtain the electronic spectra. In our calculations we use only a single point which is the sufficient condition

to consider all the orbitals and charge distribution across the entire system. Although the calculations presented here are more complete than the models adopted in the literature which take into account the electronic interaction, up to the second and third neighbors, an interesting property remains in their electronic spectra: the fractality (which is the main signature of this kind of system). We make some preliminarily considerations about the electronic gap decreasing with the increasing of the nanowire. Furthermore, we discuss the fractality trends of the spectra.

Methods

Consider a straight line of radicals (CH₂, and SiH₂) obeying a Fibonacci sequence rule. The Fibonacci chain can be obtained by an inflation rule or recursive sequence, forming a binary string that can be grown by juxtaposing two building blocks A (CH₂) and B (SiH₂). The n-th stage Sn of Fibonacci chain is generated by: Sn = Sn-1Sn-2 ($n \ge 2$), with S0 =B and S1 = A. Another way to obtain a GFS is through the recurrence relation $A \rightarrow AB$ and $B \rightarrow A$. The total number of blocks A and B in Sn is equal to the Fibonacci number Fn, and is given by the recurrence relation Fn = Fn-1 + Fn-2, with F1 = F0 = 1. The first terms of the sequence are : A, AB, ABA, ABAAB,..., where A and B are building blocks of the sequence, i. e., CH₂, and SiH₂ radicals, respectively. We adopted an initial bond length of 1.5 Å between Si - C and C - C. After a complete optimization, the final bond length found for Si-C, and C-C were around 1.87Å, and 1.53Å respectively. In the Figure 1 we show a 3D representation of the fifth generation molecule.



Figure 1. Atoms disposition in a CH2-SiH2. The atom number one is at the origin, while the atom number two is at 1.6 Å to the right of the atom one, and the same rule we apply to others terms of the Fibonacci sequence. This figure is equivalent to the ABAAB term.

Results and Discussion

In the Fig. 2, we show results obtained for the spectra of eigenenergies for each generation, and the corresponding density of states for the whole spectrum. The DOS indicates a fractal trends on the bands structures.

In the Fig. 3 we show the band gap variation with length of the chain or nanowire Fibonacci generation. There is a decreasing of the gap with the chain increasing, which is awaited property in a typical polymer. Although we have just quantum mechanics qualitative results, we can infer from the observed results, that for quasiperiodic chain, in general the gap is lower than the periodic chain for same generation, which is surprising interesting, the order of chain growth could influence the gap behavior. Further investigation with a more robust quantum mechanics method would provide a better understanding of this behavior.



Figure 2. Energy levels in function of the generation number for Fibonacci nanowire, and the corresponding to the entire density of states(DOS) for the whole spectrum.



Figure 3. Gap energy behavior for each Fibonacci generation n. Open blue circle corresponds to periodic nanowire. Open red square corresponds to Fibonacci nanowire. Figure 3. Gap energy behavior for each Fibonacci generation n. Open blue circle corresponds to periodic nanowire. Open red square corresponds to Fibonacci nanowire.

Conclusions

In summary, we investigated the Quasiperiodic CH_2/SiH_2 atomic nanowire with extended Hückel methodology. Our calculations show clearly a fractal aspect in the eigenenergies distribution with the increasing of the Fibonacci generation, i.e. the inclusion of more complex structure with four orbitals per atom does not break the main property of this system: the multifractality. Curiously there is an electronic gap reduction with the introduction of disorder through quasiperiodicity along the nanowire. Maybe this could happen due of some above mentioned Hückel method limitations. Further investigations with more precise methods would clarify this aspect.

If we compare with others models, the method applied here are more complete and could give more physical information not explored yet in the literature. We hope that the present findings described in this paper may stimulate further investigations in the quasiperiodic molecular nanowires.

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