Translocation of DNA bases sandwiched between two graphene layers: an *ab-initio* study on their energetics and molecular fingerprints.

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ABSTRACT

In this work, we studied the interactions of the complexes of a DNA base inserted between graphene layers through density functional theory (DFT) calculations. We find that there exists the negligible energy barrier as well as robust and distinguishable electronic fingerprints during the translocation of the DNA bases. Our result shows that the bilayer graphene can be a possible candidate for the future-generation of DNA sequencing device platform.

INTRODUCTION

DNA sequencing, detecting, and differentiating the four types of nucleobases in a DNA strand, adenine, cytosine, guanine, and thymine, is one of the most important goals in biology and has immense medical implications. In this effort, a promising approach is the combination of the longitudinal translocation of single-stranded DNA (ssDNA) through solid-state nanopores and the simultaneous sensing of nucleobases using transverse electron tunneling. After the initial theoretical propositions, the feasibility of tunneling-based identification has now been demonstrated through experiments. However, in these experiments that employed Au electrodes, signals from different nucleotides markedly overlapped with each other and the difficulty arises from the overadsorption of nucleobases to metallic surfaces. In this regards, the novel DNA sequencing electrodes such as graphene attracts great interest these days.[1-2]

In this study, we investigated the interaction energy and electronic signals of DNA bases with two layers of graphene electrodes, where the DNA base is sliding through.

Structural stability and electronic properties are studied through calculating the translocation energy and partial density of state (PDOS), respectively. We find that there exists the negligible energy barrier as well as robust electronic fingerprints in translocating the DNA bases. Our result shows that the bilayer graphene can be a possible candidate for the future-generation DNA sequencing device platform. [3]

This work is expected to be a valuable preceding-research for finding the novel device architecture of grapheme-based DNA sequencing sensor

Modelling and METHODS

We study four of nucleobases as shown in Fig 1(a), adenine, guanine, cytosine and thymine using local density approximation (LDA – CA) in LCAODFTLab of the EDISON Nano-physics that can calculate density functional theory (DFT).

We insert the nucleobases in replacement of middle layer in the AAA stacking of graphene layers as shown in Fig 1(b). The inter-distance, C, for the AA stacking graphene layers has been experimentally determined to be **C = 3.55 Å.** [4] Therefore, the inter-distance of our model is determined to be **C X 2 =7.1 Å**. We assumed that DNA base is sliding between two of graphene layers and calculated the relative binding energy depending on relative position [Fig.1 (c)]

We have performed the total energy calculation to find the optimized unit-cell with changing lattice constant. We have defined the unit-cell like Fig 2(a). As a result, we find that the optimized lattice parameter is **2.4902 Å** at lattice vector.

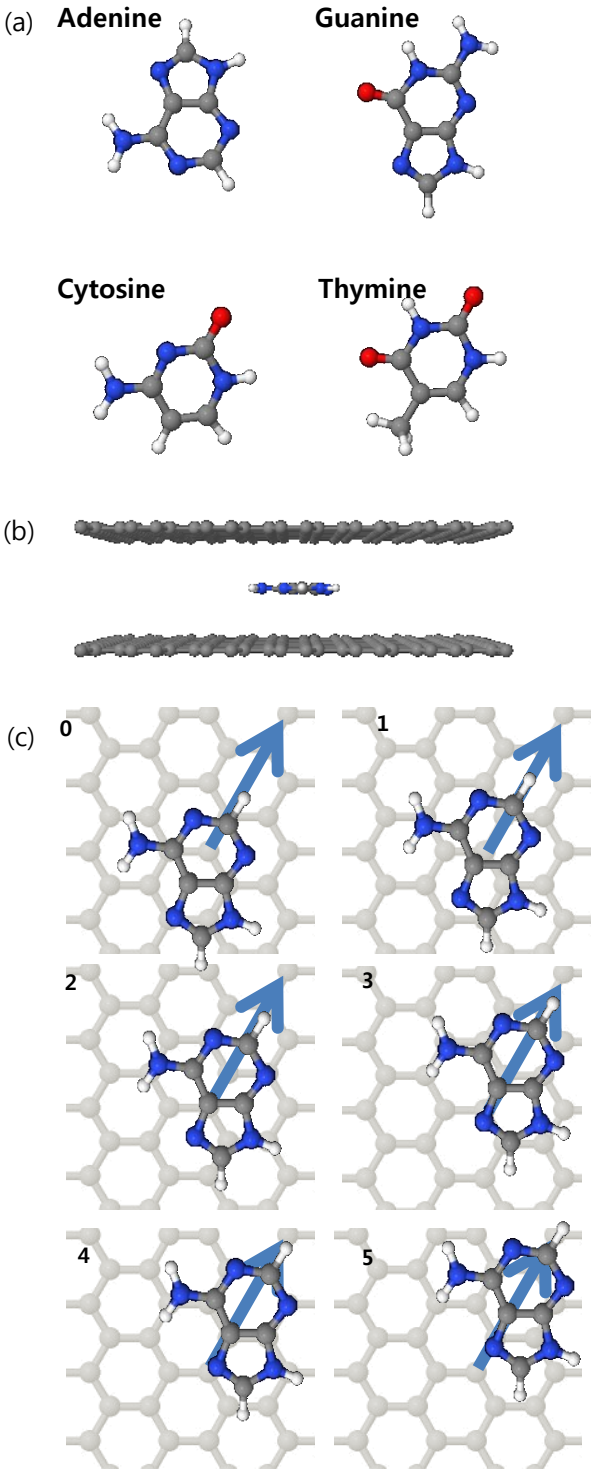

Fig. 1 (a) Four of the DNA bases. (b) Side views of atomic structure of DNA base (adenine) between the two of graphene layers. (c) The slid position of DNA base on graphene, 0,1,2,3,4 and 5.

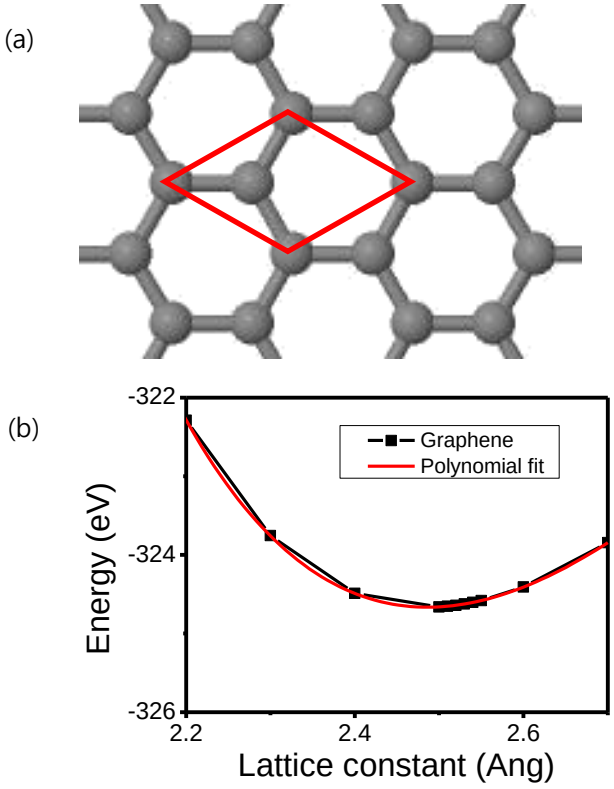

Fig. 2 (a) Graphene unit cell. (b) Cell test, the total energy with changing lattice constant.

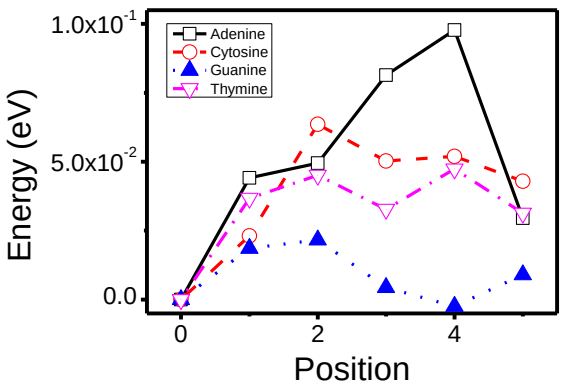

Fig. 3 The normalized binding energy of DNA base with graphene layers depending on relative position.

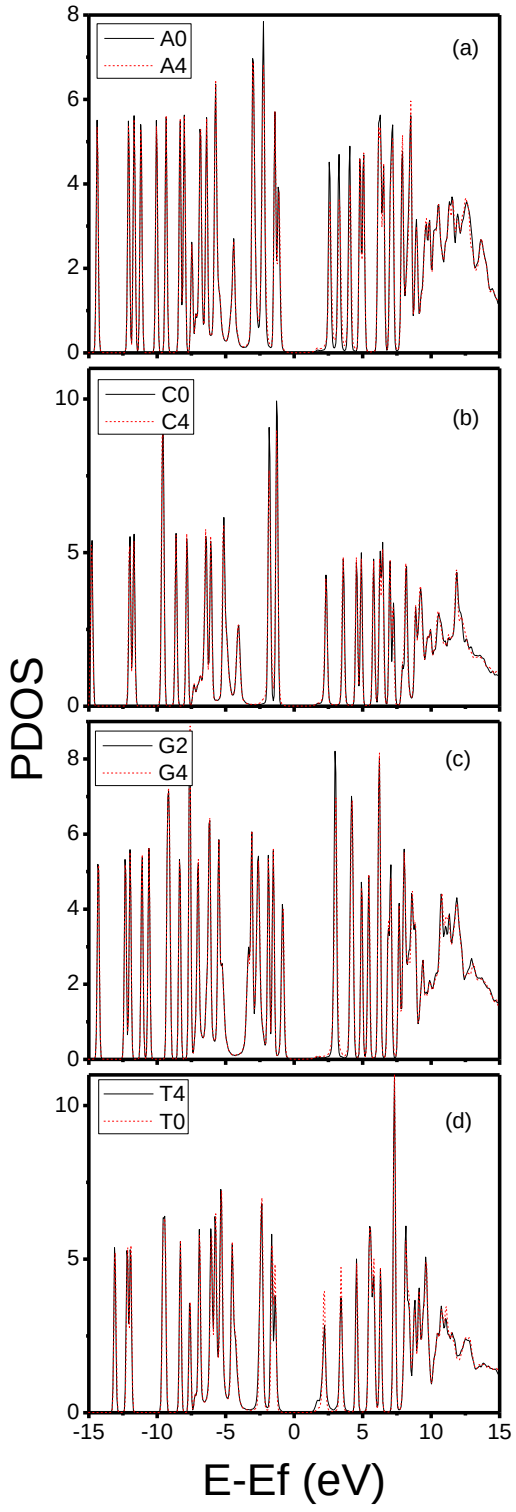

Fig. 4 The projected DOS at maximum and minimum of binding energy. (a) The position 0 and 4 of adenine. (b) The position 0 and 4 of cytosine. (c) The position 2 and 4 of guanine. (d) The position 0 and 4 of thymine.

RESULT AND DISCUSSION

We first observe the relative binding energy difference of DNA base with graphene layers depending on translocation path. For each type of bases, the lowest energy throughout the translocation path is set as zero. [Figure 3] Then the energy barrier was plotted accordingly. Among the four bases, adenine shows the highest sliding energy barrier of about 0.1eV which is expected to be easily overcome by thermal fluctuation. Therefore, for all four bases, the translocation energy barrier is negligible. This indicates that this architecture is suitable for high-speed DNA sequencing.

Then, we have studied electronic properties of the graphene with a DNA base calculating projected DOS. Figure 4 shows projected DOS diagrams at maximum and minimum of binding energy. There is no diffirence of PDOS between maximum and minimum as shown the figures. It means that regardless of the positions, we will get same electronic signal in the DNA sequencing.

In Figure 5, It is compared the PDOS of the four of DNA bases, adenine, cytosine, guanine and thymine at the position of minimum energy. We can get distinguishable signals and sense the DNA bases in the DNA sequencing.

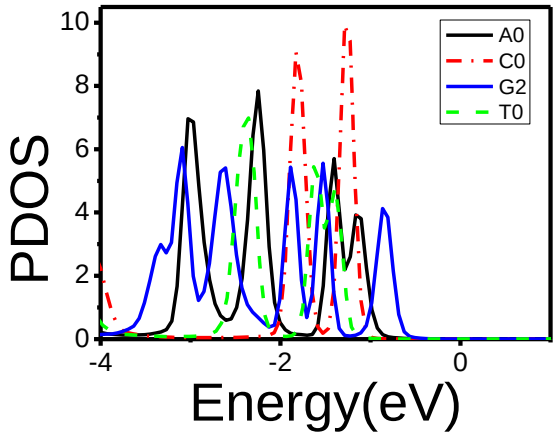

Fig. 5 Projected DOS of the four of DNA bases, adenine, cytosine, guanine and thymine at the position of bottom energy.

CONCLUSION

In summary, we studied pre-research for applying bilayer graphene to DNA sequencing sensor. In this research, we calculated translocation energies and it's PDOS diagrams using local density aproximation(LDA-CA) in LCAODFTLab of the EDISON Nano-physics which can calculte density functional theory(DFT). The energy barrier is enough negligible small and also, the noise of this signal is that in this system. We can detect the distinguishable signal of each DNA bases. We shows that this system has possibility for new DNA sequencing sensor through this research.

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