P306

Ab initio Study of Electronic Properties of n-Thiophene Molecules

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Introduction

Thiophene molecule (C_4H_4S) is a heterocyclic aromatic compound which is shown in Figure1. Thiophene heterocyclic compounds are important in organic chemistry. Among the important common applications of this type of polymers is using in the manufacture of solar cells[1], organic light emitting diodes(OLED)[2], spintronics, sensors and other electronic devices. In this study we investigate the electronic and structural properties of n- thiophene molecules.

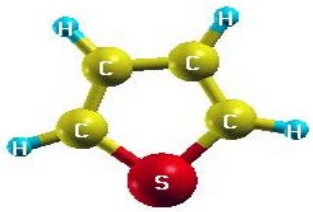

Fig. 1. Thiophene molecule structure

Methods

The electronic structure is calculated by using density functional theory (DFT)[3], as implemented in SIESTA code[4]. The cut-off energy is set at 500 Ry and the generalized gradient approximation (GGA) is used as exchange-correlation functional through this work.

Results and Discussion

The electronic structure of the isolated n- thiophene for the molecules with different lengths ranging from n=1 up to n=10 thiophene rings are calculated. The calculated electronic band structure of these molecules is shown in Figure 2. The HOMO-LUMO gaps for all n-thiophene molecules are calculated and the results are displayed in Figure3. The results revealed that the HOMO-LUMO gap decreased by increasing the number of thiophene

rings. The total energies of n-thiophene molecules based on the number of rings are displayed in Figure 4. which indicates that structures with higher rings are more stable.

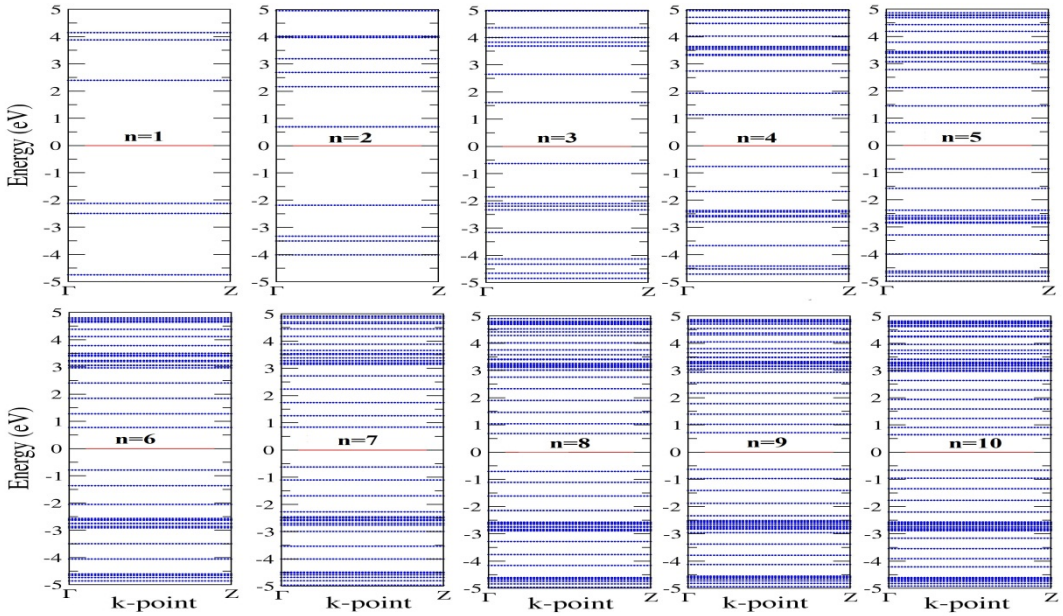

Fig. 2. Electronic band structures of n-thiophene molecules.

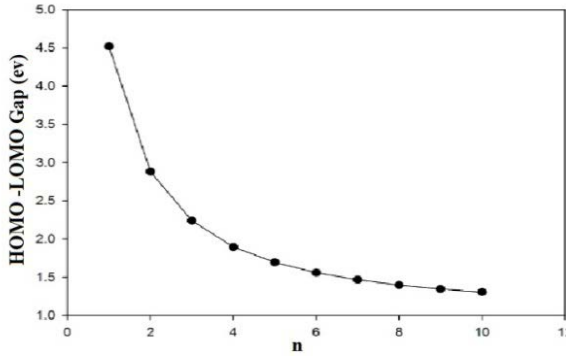

Fig. 3. HUMO-LUMO Gap vs number of rings (n).

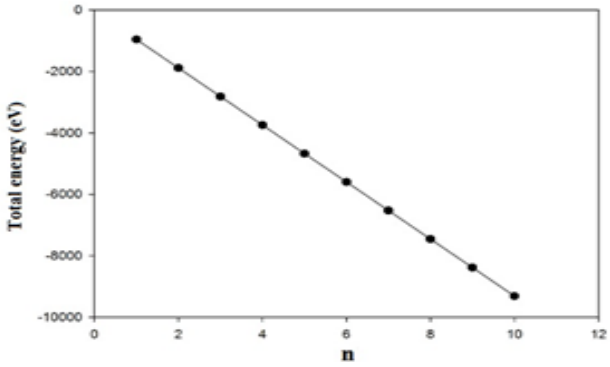

Fig.4. Total energy vs number of rings (n).

Conclusions

The electronic properties of n-thiophene molecules with different rings were calculated based on density functional theory. The results revealed that by increasing the number of thiophene rings the HOMO-LUMO gap and the total energy decreases and the structures with higher rings were more stable.

References

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