

Density Functional Theory study of convergence in the HOMO –LUMO Gap of fluorene-thiadiazole oligomers

Daniel Glossman-Mitnik¹, Norma Flores-Holguín¹, and Luz María Rodríguez-Valdez²

¹Departamento de Simulación Computacional y Modelado Molecular - CIMAV, SC M. de Cervantes 120 - Comp. Ind. Chihuahua - Chihuahua, Chih. 31109, México ²Facultad de Ciencias Químicas - Universidad Autónoma de Chihuahua Nuevo Campus Universitario - Chihuahua, Chih. 31125 - México

e-mail: norma.flores@cimav.edu.mx

The lower manufacturing costs of semiconductor organic compounds and their physical and chemical properties make them a novel option as electronic materials in areas not covered by inorganic compounds. They present a number of advantages: easy fabrication, large area, flexible and light weight devices [1,2].

In recent years thiophene-based electronic materials have been extensively investigated. The ease in chemical modification of their structures can potentially allow us to fine-tune their optical and electronic properties [3]. These properties have a short relationship with the double bonds in the structure and the introduction of substituent in specific positions. In this study an addition of N in the 3 and 4 position was made in the thiophene ring to produce 1,3,4-thiadiazole and fluorene is added at both sides of the chain.

The objective of this work is to predict the HOMO-LUMO Gap of these series of fluorene-thiadiazole oligomers increasing the chain and extrapolating the linear curve of the band gap against the reciprocal of monomeric units ($1/n$) to find the exact length distribution and geometry of long-length conducting polymer.

All calculations of these oligomers was performed using the Gaussian 03 program with the Density Functional Theory, B3LYP and 6-31G(d).

References

1 Mozer, A. J.; Sariciftci, N. S. C R Chim 2006, 9, 568.

2 Nazeeruddin, M. K.; De angelis, F.; Fantacci, S.; Selloni, A.; Visca, G.; Graätzel, M. J Am Chem Soc 2005, 127, 16835.

3S. Hotta, Molecular conductive materials, polythiophenes and oligothiophenes in :H.S. Nalwa (ed.), Handbook of Organics Conductive Molecules and Polymers, Vol 2, Wiley, Chinchester, 1997.