

# Study of the behavior of polyvinylidene fluoride (PVDF) under the action of electric field using semi-empirical methods (PM3)

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Abstract. Piezoelectric material has the property of converting energy from the mechanical pressure of an external body into electrical energy on the piezo-structure, providing a strong potential source for renewable energy. Our aim in this article is to explore the properties of polyvinylidene fluoride polymer under the influence of an electric field. In sense to understand the behavior of integer polymer, we started to simulate the optimization of several small sizes (monomer, dimmer, trimer and tetramer) of this polymers subjected to uniform electric fields in the direction of the electric dipole applying a external electric field and analyzing the displacement of electrical charges. For this optimization of this polymer we used PM3 semi-empirical methods applying electric field applications. These results elucidate the behavior of electrical charges of an organic piezoelectric material under the action of external and uniform electric field.

# Key words

Piezoelectric materials, PVDF, Semi-empirical methods, PM3 electrical field.

# 1. Introduction

Nowadays the search for new sources of energy has increased the development of the technologies that may produce devices capable of several types of energy into electrical currents. One of these types of engines is those based on piezoelectric materials.

In 1969, Kawai [1] discovered the piezoelectric effect on polymer polyvinylidene fluoride (PVDF), since then the molecule and his co-polymers have been well investigated. One approach that has established itself from the most detailed researches is the use of piezoelectric materials as actuators and transducer of sensors [2], by transforming the pressure made on them into electric pulses these materials are of great importance for the industry of devices supported on this principle.

The PVDF [3] is a piezoelectric polymer applicable to many systems. The PVDF has unique features, such as an excellent mechanical behavior, lightweight, great stress without structural fatigue, corrosion resistance, easy processability on dielectric thin films [4] and the most important, design of flexible architecture by molecular research. PVDF is a specialty plastic material in the fluoropolymer family. PVDF with melting point of around 177°C.

Other possible applications are piezoelectric bio-sensors which represent an economic approach suitable for the detection of a variety of bio-molecules. However, there are technical difficulties to use conventional piezoelectric crystals limiting their potential applications. Piezoelectric polymers and its co-polymers are considered as a favorable choice on the fabrication of different types of sensors, due to its low cost, lightweight and facility in the formation of delicate forms. [5]

Until the present moment were cataloged four crystalline structures of the monomers, these being denominated as  $\alpha$ ,  $\gamma$ ,  $\beta$  and  $\delta$ , however the main interest revolves around the  $\beta$ , because it has a good utility for industry. [6]

To reveal the effect of the electric field on to the structure and the electric properties of PVDF, as well as the transformations of phases, many aspects must be taken into account, including the origin of the stability in a PVDF, the energy barrier, the possibility of a transition between different phases, the effect of different electric fields on the geometry and the dependence of the properties with the geometry. Based on this propose some researches have been performed different simulation methods. [4-6]

Piezoelectric material could be used in shoes to storage electric energy in a small personal battery from the pressure due to weight of the person. It could also be used in streets and sidewalks to receive energy from walking people [7] and road traffic [8-9]. Also, piezoelectric materials have been used in car brakes [10] to accumulate energy in the battery of the car.

Thus, our objective here is to study the behavior of electrical properties of fragments of PVDF when exposed to several electric field of constant module using optimization of PM3 semi-empirical methods.

#### 1. Methodology

To better understand the properties of PVDF, we have four different sizes of this polymer starting from one molecule (monomer) to four (tetramer), performing the optimization of the static structure under influence of an uniform electric field. In order to gain a deep insight on electrical charge properties of the polymer each interaction was made by several external electric field values.

The variations of electric charge under uniform electric field was calculated applying the field in the direction of electric polarization of the monomer (N1), dimmer (N2), trimer (N3) and tetramer (N4) of PVDF. Because of its faster convergence between the algorithms available, evaluated the simulations utilizing a PM3 semi-empirical method, with the Polak-Ribiere algorithm (a technique of conjugated gradient which uses one-dimensional searches) being used for the optimizations using Hyperchem 7.5 program package [11].

## 2. Results



Fig. 1. Simulation of electrical charge of PVDF versus external electric field value.

Figure 1 presents the variation of the electrical charge of PVDF with uniform electric field using optimization of PM3 semi-empirical method. Also, this figure displays that the electric charge induced for the monomer has a very small value. For the dimmer, the electrical charge increases with non linear form because there are more atoms in this molecule than the monomer. In case of the trimmer, we have a behavior almost linear, and more electrical charges are changing of place of the position of the electric polarization between Fluor and hydrogen atoms of PVDF. For tetramer case, we have a gap between the negative and positive values of electric field; this it shows a special resonant travel of electrons between the geometric positions of the Fluor and hydrogen atoms of this electric polarization. It should be kept in mind that there is a well-knowledge PVDF experimental peak in 0.002 a.u of electric field.

## 4. Conclusion

That molecule of PVDF, beginning from monomer to the tetramer, interacting under a uniform electric field during this optimization presented electrical charge variation between Fluor and hydrogen atoms. We verify that the electric charge *versus* electric field changes with the size of the polymer, thus, for the monomer, dimmer, trimmer and tetramer the negative and positive values of electric field are continuum, except for the tetramer case, where there is a resonance between Fluor and hydrogen atoms for small values of negative and positive electric field.

From the results above we also conclude that the stability of the polymer becomes noticeable after the fourth multiple of the monomer.

From these remarks, we can understand deeply the behavior of the polymer during the process of formation and how its stability increases with the size of the molecule.

Due to its flexibility and easy applicability, PVDF is a proponent material in the establishment of several types of devices that can provide renewable energy from different sites, for example, shoes, streets, sidewalks and car brakes.

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