ISSN : 2249 - 8877 Volume 3 Issue 4

Trade Science Inc.

Research & Reviews On Polymer

Full Paper

RRPL, 3(4), 2012 [117-120]

First-principles study of ethylene tetrafluoroethylene

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ABSTRACT

First-principles calculations based on Density Functional Theory has been employed to simulate the structure of Ethylene tetrafluoroethylene. Structural parameters have been measured. Electron density of states, Dielectric constant and phonon modes have been computed and the results have been reported in the present paper. Phonon modes indicate that the structure is highly stable. Electron density of states indicate that the material is a very good insulator.

KEYWORDS

Ethylene tetrafluoroethylene;
First-principles calculations;
Electron density of states;
Dielectric constant;
Phonon modes.

INTRODUCTION

Ethylene tetrafluoroethylene, ETFE is a fluorine based translucent plastic material and its systematic name is poly (ethylene-co-tetrafluoroethylene). It is designed to have high corrosion resistance and strength over a wide temperature range. ETFE has a very high melting temperature, excellent chemical, electrical and high energy radiation resistance properties[1].

ETFE is used in the nuclear industry for tie or cable wraps, and in the aviation and aerospace industries for wire coatings. This is due to its better mechanical toughness than poly tetrafluoroethylene (PTFE), it finds several applications. In addition, ETFE exhibits a high-energy radiation resistance and can withstand moderately high temperatures for a long period of time[2].

Due to its high temperature resistance ETFE is also used in film mode as a mold release film. ETFE film is used in aerospace applications such as carbon fiber curing as a release film for molds or hot high pressure plates.

Compared to glass, ETFE film is 1% the weight transmits more light and costs 24% to 70% less to install. It can withstand huge loads of about 400 times its own weight. It is easy to clean its sheets due to its non-stick surface and it is recyclable. On the other hand it is prone to punctures by sharp edges, therefore it is mostly used for roofs. In sheet form as commonly employed for architecture, it is able to stretch to three times its length without loss of elasticity. Employing heat welding, tears can be repaired with a patch or multiple sheets assembled into larger panels. ETFE has an approximate tensile strength of 42 N/mm^2, with a working temperature range of 89 K to 423 K[3].

Any little modification in the structure and composition of a Polymer will bring in sufficient changes in the properties of the polymer[4,5]. Thus it is important to study the structure of the Polymers and look at the parameters which can be altered to get a better material for technological applications. First-principles calculations based on Density Functional Theory[6] has been proved to be an effective tool in the study of structural, electronic and dielectric properties of polymers[7,8]. With this in view, structure of ETFE has been simulated using

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First-principles calculations based on Density Functional Theory and computation of Electronic density of states, Dielectric constant and phonon modes have been done and the results have been reported in the present paper.

COMPUTATIONAL DETAILS

Several codes are available for the theoretical structure simulation[9]. We use plane wave self consistent field (PWSCF)[10] implementation of density functional theory (DFT), with a Local density approximation (LDA)[11] to exchange correlation energy of electrons and ultrasoft pseudopotentials[12], to represent interaction between ionic cores and valence electrons. Kohn-Sham wave functions were represented with a plane wave basis with an energy cutoff of 40 Ry and charge density cutoff of 240 Ry. Integration over Brillouin zone was sampled with a Monkhorst-Pack scheme[13] with appropriate k point mesh and occupation numbers were smeared using Methfessel-Paxton scheme[14] with broadening of 0.003 Ry. The structure was relaxed to minimize energy.

RESULTS AND DISCUSSION

Structure of ETFE

Completely relaxed structure of the ETFE was observed using the XCrySDen software[15] and the structure as seen from different directions have been given in Figures 1 - 4.

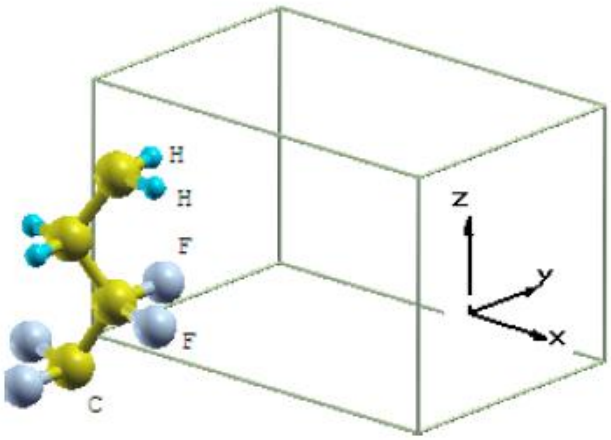

Figure 1 : Structure of ETFE as viewed along a random direction

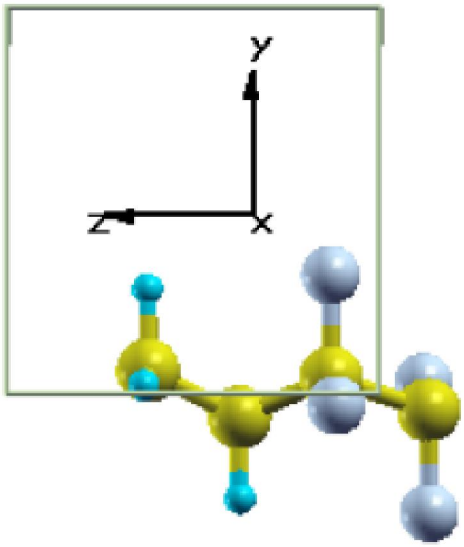

Figure 2 : Structure of ETFE as viewed along X-axis

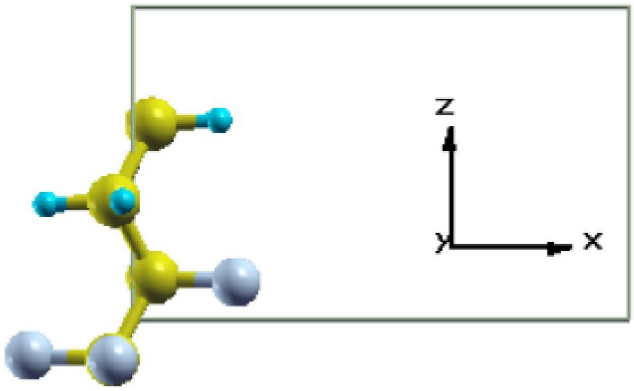

Figure 3 : Structure of ETFE as viewed along Y-axis

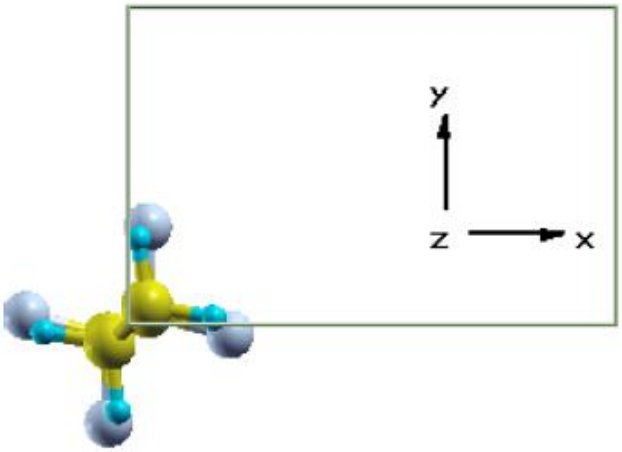

Figure 4 : Structure of ETFE as viewed along Z-axis

Structural parameters of the simulated structural pattern of ETFE are given in TABLES 1, 2 and 3.

EDOS calculation

Electron Density of States (EDOS) have been computed in the polymer ETFE using Electronic structure calculation code of Quantum espresso and the same is shown in Figure 5. The material shows a large band gap of 6.74eV, which proves the high insulator nature of this polymer.

TABLE 1 : Bond lengths in ETFE

Bond	Bond length (Å)
H - C	1.101
F - C	1.381
C - C	1.505

TABLE 2 : Bond angles in ETFE

Bond	Bond angle (degree)
H - C - H	108
H - C - C	111
C - C - C	111 to 115
F - C - F	106
F - C - C	107

TABLE 3 : Other structural parameters in ETFE

Parameter	Value
H – H dist	1.777 Å
F – F dist	2.207 Å
a	7.955 Å
b	5.200 Å
c	5.000 Å
Vol of unit cell	206.83 Å^3

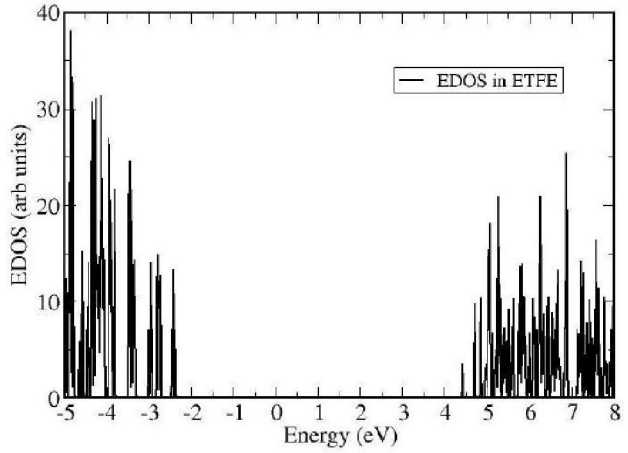

Figure 5 : Electron density of states in ETFE

Dielectric constant and phonon modes

Dielectric constant of the polymer has been computed and it comes out to be 1.431, 1.580 and 1.655 along X, Y and Z axes respectively and the average value comes out to be 1.555. The computed phonon modes at the gamma point are all positive and range from 16cm^{-1} to 3032cm^{-1} showing that the simulated structure is highly stable.

CONCLUSIONS

First-principles calculations based on DFT has simulated a highly stable structure of ETFE. EDOS calculations show that the polymer has a large band gap of 6.74eV. The material has an average Dielectric constant of 1.555 from the electronic contribution. Phonon modes range from 16cm^{-1} to 3032cm^{-1} showing that the simulated structure is highly stable. Present study reveals that the First-principles calculations based on DFT can be effectively employed to study the electronic and dielectric properties of the polymer ETFE.

ACKNOWLEDGEMENTS

Author would like to thank the University Grants Commission, India for the financial assistance under MRP Scheme [MRP(S)-798/10-11/KAMY022/UGC-SWRO] to carry out this work. Author is also thankful to Prof. Umesh V. Waghmare, Theoretical Sciences Unit of JNCASR, Bangalore for his guidance.

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