Electronic and Physical Studies for Teflon FEP as a Thermal Control in Low Earth Orbit Reinforced With ZnO and SiO₂ Nanoparticles

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Abstract

Fluorinated Ethylene Propylene (Teflon FEP) is used as external layer thermal insulator for Hubble Space Telescope (HST) and on the outside surfaces of space crafts in the low earth orbit (LEO). Teflon FEP was eroding as a result of exposure to Atomic Oxygen (AO) and different electromagnetic waves such as Ultraviolet radiation and X-ray. Model molecules were used to simulate Teflon FEP and its interaction with other nanoparticles such as ZnO and SiO₂. Density functional theory (DFT) was used to calculate model structures using B3LYP/LAN2DZ model. Molecular Electrostatic Potential as contour, band gap energy and total dipole moment were computed for all models. Thermal stability properties were also studied for Teflon FEP both individually and interacted with ZnO and SiO₂. Results showed that a layer of OZn and SiO₂ on Teflon FEP, especially Teflon FEP+OZn+OSiO structure, improves the physical, chemical, thermal, and electrical stability of Teflon FEP, potentially acting as a corrosion-inhibiting layer.

1. Introduction

Polymers applied for space applications are now termed as space polymers. Space polymers including Teflon FEP, Kapton polyimide, and poly (methyl methacrylate) can be exposed to a reversal of incident photons, atoms and/or atomic and vacuum ultraviolet (VUV) ions (Moser 2008). Teflon FEP is often used as an external surface of multilayer insulation (MLI) blanket on the Hubble Space Telescope (HST) (Dever 2000; De Groh et al. 2004). Through space shuttle operation missions (SM) to HST, cracks in thickness were found in FEP layers. The material that was sent to Earth for study showed symptoms of significant degradation (De Groh 2003; Minton et al. 2010; Yeong 2017). Aging of Teflon FEP, has also been recorded (Jucius 2011; Jucius et al. 2010, Bhagat 2015). It was found that Al₂O₃ atomic layer deposition (ALD) coatings could effectively shield polymers against oxygen-atom erosion and VUV corrosion, because Al₂O₃ ALD coatings shield the corresponding polymers from atomic-oxygen attacks (Yeong 2017). Moreover, the modification with TiO₂ coatings protects the surfaces from VUV-induced corrosion (Chao 2019). Teflon FEP appears to be very structurally comparable to Polytetrafluoroethylene (PTFE) which is a well-known polymer with remarkable mechanical strength and electrical properties, low impact resistance and thermal stability, as well as other attributes including low surface energy and chemical stability, and is a cost-effective material (Galante 2010). The outstanding mechanical and physicochemical properties of PTFE served as a framework for the addition of ZnO nanotubes (Shabannia 2014), and enabled for the efficient creation of flexible sensors (Agrawal 2017). The possibility of developing nanoscale photodetectors for nano-optics applications were exhibited for ZnO nanotubes, which were successfully produced using a wet simple preparation method on such Teflon substrate (Farhat 2015). Silica is a ceramic material with unique properties such as high strength, corrosion inhibition and excellent insulation. Because of these impressive characteristics, SiO₂ and PTFE are particularly well suited to a wide range of technical applications. Superhydrophobic structures have shown to be an exceptional asset in variety of applications, including self-cleaning (Plirdpring 2020), and protective properties such as anti-icing (Liang 2018) and anti-corrosion characters (Zhu 2020). Studies on PTFE filled with SiO₂ demonstrated that SiO₂ filling reduces PTFE porosity deformation while enhancing the material's mechanical properties and toughness (this sentence needs references). Furthermore, it was reported that increasing the quantity of SiO₂ increased the

mechanical strength of PTFE/SiO₂ matrix (Chen 2007). PTFE/SiO₂/Epoxy composites were also studied (Shen 2015) it was as similar as PANI/PTFE/GO composites, which have registered an improvement in the electrical properties used for the fabrication of electrochemical devices (Badry 2020). ZnO/SiO₂/PTFE film on glass has been developed with anti-icing characteristics, corrosion resistance and insulation properties, with the film's corrosion resistance and insulating capabilities greatly enhanced owing to the addition of SiO₂ medium to the specimen, which gives a new concept for the design of an insulating surface on glass that serves as an anti-icing surface (Ruijin 2017).

Molecular modeling is a series of computational calculations that assess the electronic properties of chemical structures with various interactions by measuring parameters such as HOMO/LUMO band gap energy (ΔE), total dipole moment (TDM) and molecular electrostatic potential (MESP), that describe the electronic properties and reactivity of the studied structure. DFT: B3LYP/LANL2D is the suitable basis set for studying the matrix of the nanoparticles/polymers interactions (Lee 1988; Miehlich et al. 1989; Becke 1993, Elhaes 2018). Furthermore, Quantitative Structure Activity Relationship (QSAR) is a tool for studying molecular behaviour that may be used to explore the bioactivity and physicochemical properties of novel compounds in the electrical, chemical, and biological sciences (Abdelsalam 2018; Abdelsalam et al. 2019).

The present work is conducted using DFT simulations to assess the electronic properties and thermal stability of Teflon FEP interactions with metal oxides (MOs), such as ZnO and SiO₂. The interaction of Teflon FEP structures with ZnO, SiO₂, and a combined effect of the two MOs was investigated. B3LYP/LANL2DZ was used to calculate TDM, MESP, and ΔE . For the same interactions, QSAR descriptors were developed.

2. Calculations Details

Model molecules were designed as four Teflon FEP units. Teflon FEP was then interacted with ZnO and SiO₂. Design and calculations were implemented using the GAUSSIAN09 software at Molecular Spectroscopy and Modeling unit, National Research Centre, Egypt. All model structures were studied using DFT theory at B3LYP level using the LANL2DZ basis set. The values of ΔE , TDM and MESP (as contour) were all calculated using the same level of theory. QSAR descriptors were calculated using semiempirical method at PM6 level of theory.

3. Result And Discussion

3.1. Teflon FEP model structures and HOMO/LUMO orbital distribution:

The chemical composition of Teflon FEP originally recommended that Teflon FEP gets connected with ZnO through various sites to decide the correct site of interaction of Teflon FEP with MOs, since the interaction of Teflon FEP with other chemical structures and its active sites are unpredictable or unknown. The contact of Teflon FEP with ZnO occurs at numerous sites due to the oxygen atom of ZnO (Ezzat 2019), since MOs interact with other chemical structures through the oxygen atom. As shown in Fig. 1, the optimized structures and their HOMO/LUMO orbital distribution of OZn interaction with Teflon FEP were explored at different

places (P1, P2, P3, and P4), such that the interaction of OZn with Teflon FEP was simulated as an adsorption state interaction. The main parameters for assessing the electrical properties of materials are TDM and ΔE . The relationship between the increase in TDM and the decrease in ΔE can be used to predict the site through which Teflon FEP should interact with OZn. Table 1 shows that the interaction of Teflon FEP with OZn resulted in a change in the values of TDM which increased from 0.669 to 7.4256, 5.4734, 5.3226 and 4.4706 Debye for Teflon FEP + OZn (P1, P2, P3 and P4) respectively, while ΔE decreased from 7.4391 to 2.3043, 2.2134, 1.7799 and 2.2466 eV for Teflon FEP + OZn for P1, P2, P3 and P4 respectively. The lowest value of ΔE was recorded for Teflon FEP + OZn P3 which, therefore, represents the most suitable position of interaction for Teflon FEP.

Table 1

DFT:B3LYP/LANL2DZ calculations for Teflon FEP and Teflon FEP interaction with OZn through different sites of Teflon FEP structure as TDM (Debye) and ΔE (eV).

Structure	TDM	ΔE
Teflon FEP	0.669	7.4391
Teflon FEP + OZn P1	7.4256	2.3043
Teflon FEP + OZn P2	5.4734	2.2134
Teflon FEP + OZn P3	5.3226	1.7799
Teflon FEP + OZn P4	4.4706	2.2466

Accordingly, 4 units of Teflon FEP were interacted with 4 ZnO, SiO₂ and a combination of the ZnO and SiO₂. In the case of the interaction of a combination of ZnO and SiO₂ with Teflon FEP, the interaction was supposed to happen as sandwich; once as Teflon FEP + 4OZn + 4OSiO and once as Teflon FEP + 4OSiO + 4OZn, and other as ZnO and SiO₂ together interacted with Teflon FEP atom by atom (Teflon FEP + 4OZn/4OSiO) as illustrated in Fig. 2. TDM and ΔE were calculated for the different proposed types of interaction. TDM increased from 0.669 Debye of Teflon FEP alone to 7.4534, 21.2799, 12.2910, 13.2651 and 5.7131 Debye for Teflon FEP + 4ZnO, Teflon FEP + 4OSiO, Teflon FEP + 4OZn + 4OSiO, Teflon FEP + 4OSiO + 4OZn, and Teflon FEP + 4OZn/4OSiO respectively as illustrated in Table 2. Moreover, ΔE decreased for the same structures from 7.439 to 0.5200, 0.5007, 0.2195, 0.5606 and 0.3135 eV respectively. The lowest value of ΔE observed was for Teflon FEP + 4OZn + 4OSiO which is an indication for the most probable interaction to occur, which enhanced the electrical properties of the Teflon FEP.

Table 2
DFT:B3LYP/LANL2DZ calculations as TDM (Debye)
and band gap energy ΔE (eV) for Teflon FEP and
Teflon FEP interacted with 4 ZnO, SiO₂ and a
combination of the two MOs.

Structure	TDM	ΔE
Teflon FEP	0.669	7.439
Teflon FEP+ 4 ZnO	7.4534	0.5200
Teflon FEP + 4 OSiO	21.2799	0.5007
Teflon FEP + 4OZn + 4OSiO	12.2910	0.2195
Teflon FEP + 4OSiO + 4OZn	13.2651	0.5606
Teflon FEP + 4OZn/4OSiO	5.7131	0.3135

3.2. Molecular Electrostatic Potential (MESP):

In order to evaluate the interaction identity of nucleophilicity, MESP was investigated using LANL2DZ basis set for the implemented Teflon FEP structure using the DFT method. The MESP maps for Teflon FEP, Teflon FEP + 4ZnO, Teflon FEP + 4OSiO, Teflon FEP + 4OZn + 4OSiO, Teflon FEP + 4OSiO + 4OZn, and Teflon FEP + 4OZn/4OSiO are shown in Fig. 3. The MESP maps show the calculation of neighbouring charges, nucleus and electron concentration at a given location. The MESP map is classified as red < orange < yellow < green < blue. The colour difference in the MESP map, which is red, indicates the lowest MESP level while blue indicates reaching the maximum MESP value. As shown in Fig. 3, the MESP maps for all connections appear coloured with intermediate colours between red and blue, which represents less electrostatic repulsion and indicates that there is still no possibility of interacting with other chemical structures, thus reflecting more chemical stability.

3.3. Quantitative Structure Activity Relationship (QSAR):

QSAR descriptors total energy (TE), heat of formation (HF), ionization potential (IP), logarithm of the partition coefficient (log P), polarization, molar refractivity (MR) and molecular weight (MW) were calculated for Teflon FEP and Teflon FEP interactions with MO as Teflon FEP + 4 ZnO, Teflon FEP + 4 OSiO, Teflon FEP + 4OZn + 4OSiO, Teflon FEP + 4OSiO, Teflon FEP + 4OSiO + 4OZn and Teflon FEP + 4OZn as shown in Table 3. TE is reported to characterize the stability upon the mechanism but whenever TE decreases, the structure is described as more durable. TE values of Teflon FEP + 4ZnO, Teflon FEP + 4OSiO, Teflon FEP + 4OSiO, Teflon FEP + 4OZn + 4OSiO, Teflon FEP + 4OSiO + 4OZn and Teflon FEP + 4OZn/4OSiO were - 21251.090, -22705.140, -24230.924, -25747.075, -25709.596 and - 23487.043 eV respectively, indicating very stable structures.

HF is a fundamental thermal descriptor that represents the energy generated as heat when atoms, existing at theoretically infinite distances, connect and build a molecule. Although HF is a concern, it could be explained by the variation in enthalpy during the creation of a single mole of a material from its components in its normal and complete equilibrium under standard atmospheric conditions at a particular temperature. HF

values for Teflon FEP + 4ZnO, Teflon FEP + 4OSiO, Teflon FEP + 4OSiO, Teflon FEP + 4OZn + 4OSiO, Teflon FEP + 4OSiO + 4OZn and Teflon FEP + 4OZn/4OSiO were - 1570.764, -1838.877, -2292.065, -2726.749, -2488.378 and - 2042.500 respectively, reflecting the production of a small amount of energy for Teflon FEP + 4OZn + 4OSiO.

The following descriptor is the IP which characterizes the reactivity of the compound and is defined as the energy required for the compound to also be ionized, meaning that the lower the IP value, the higher the reactivity of such compound. Results indicated no significant differentiation between the IP values that measured - 12.980, -9.759, -11.684, -9.450, -11.074 and - 9.851 for Teflon FEP, Teflon FEP + 4 ZnO, Teflon FEP + 4 OSiO, Teflon FEP + 4OZn + 4OSiO, Teflon FEP + 4OSiO + 4OZn and Teflon FEP + 4OZn/4OSiO respectively. The increased IP values confirm that the reactivity of the new structures is quite low, with the lowest reactivity obtained was for Teflon FEP + 4OZn + 4OSiO.

Log P is a definition of the hydrophilicity of the chemical substance. Log P is the ratio of the concentration of a substance dissolved in, for example, an organic solution to its concentration dissolved in an aqueous solvent at equilibrium. As a consequence, positive log P values are corresponding to hydrophobic compounds, while negative values are corresponding to hydrophilic compounds. All suggested models resulted in positive log P values, indicating that the compounds are hydrophobic, chemically soluble and are not affected by the surrounding medium.

The final QSAR descriptor is polarizability which is described as a basic property that defines how the chemical structure could be polarized in response to variation forces, which reflects the reactivity of the structures influenced by their volume. In fact, MR is a descriptor which determines the total polarization of a mole of the substance, such that the higher the molar refractivity, the higher the reactivity of the substance.

The obtained results support the theory that a layer of OZn and SiO₂ on Teflon FEP, in the form of Teflon FEP + OZn + OSiO, improves the physical, chemical, thermal, and electrical stability of Teflon FEP, which might serve as a corrosion-inhibiting layer for Teflon FEP that is prone to corrosion during space missions.

Table 3

QSAR descriptors as Total Energy (eV), Heat of formation (HF), Ionization potential (eV), Log P, Polarizability, Molar refractive (MR), molecular weight (MW) calculated at PM6 level for Teflon FEP and Teflon FEP interacted with 4ZnO, 4SiO₂ and a combination of both MOs.

Sample	TE	HF	IP	Log P	Polarizability	MR	MW
Teflon FEP	-21251.090	-1969.435	-13.328	12.801	28.228	1002.166	802.136
Teflon FEP + 4OZn	-22705.140	-1838.877	-9.759	11.396	53.506	1327.800	1327.800
Teflon FEP + 4OSiO	-24230.924	-2292.065	-11.684	9.990	44.738	1242.503	1242.503
TeflonFEP + 4OZn + 4OSiO	-25747.075	-2726.749	-9.450	8.584	55.772	1568.137	1568.137
TeflonFEP + 4OSiO + 4OZn	-25709.596	-2488.378	-11.074	8.584	58.688	1568.137	1568.137
Teflon FEP + 4OZn/4OSiO	-23487.043	-2042.500	-9.851	10.693	46.500	1285.151	1285.151

4. Conclusion

Molecular modelling at DFT level using B3LYP/LAN2DZ basis set can be efficiently applied to investigate the changes in the electronic behavior of the model molecules representing Teflon FEP and Teflon FEP interacted with nanoparticles of ZnO, SiO₂, and a combination of both MOs. The numerous parameters studied for all the proposed structures, including the ΔE , MESP as a contour, and even the thermal stability properties reflected by QSAR descriptors indicated that the interaction between Teflon FEP and MOs showed that a coating of OZn and SiO₂ on Teflon FEP, in the form of Teflon FEP + OZn + OSiO, increases the stability of all the properties under investigation, thus qualifying this coating to be a potential upgrade for Teflon FEP as a corrosion-inhibiting layer for space missions.

Declarations

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Figures

Figure 1

Optimized and HOMO/LUMO orbital distribution of Teflon FEP and Teflon FEP with MOs such as OZn as (a) Teflon FEP; (b) Teflon FEP+OZn P1; (c) Teflon FEP+OZn P2; (d) Teflon FEP+OZn P3; (e) Teflon FEP+OZn P4

Figure 2

Optimized and HOMO/LUMO orbital distribution of Teflon FEP and Teflon FEP interaction with 4 ZnO, SiO₂ and a combination of the two MOs. (a) Teflon FEP; (b) Teflon FEP+40Zn; (c) Teflon FEP+4 OSiO; (d) Teflon FEP+40Zn+40SiO; (e) Teflon FEP+40SiO+40Zn; (f) Teflon FEP+40Zn/40SiO

Figure 3

Teflon FEP and Teflon FEP interaction with ZnO, SiO₂ and a combination between the two MOs together MESP as (a) Teflon FEP; (b) Teflon FEP+4 ZnO; (c) Teflon FEP+40 SiO₂; (d) Teflon FEP+40 ZnO+40 SiO₂; (e) Teflon FEP+40 SiO₂+40 ZnO; (f) Teflon FEP+40 ZnO/40 SiO₂