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# Atomistic study of adhesion of PU/PTFE coating on aluminium oxide surface

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## ABSTRACT

The effectiveness of coatings depends upon various factors and adhesion of the coating to a metallic surface is one of them. Polyurethane (PU) and polytetrafluoroethylene (PTFE) are widely used polymeric coatings for the protection of metallic surfaces. The adhesion of PU and PTFE films on the aluminium oxide substrate is investigated by employing MD simulations. The effect of temperature variation on both the polymeric films has been also studied. Results depict that as the temperature increases the adhesion energy of both the polymers increases in the range from 273.15 K to 298 K. However, there is no such applications of these polymeric coatings at higher temperature like 548 K, the interaction energy is also calculated at 548 K to predict the behaviour of these polymers at elevated temperatures. PU was found to be more thermally stable compared to PTFE. Moreover, PU adhesion with the aluminium oxide surface was much greater when compared to PTFE which possibly resulted from the existence of oxygen atoms in PU which are responsible for greater adhesion between polymer and metal surface.

## ARTICLE HISTORY

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## KEYWORDS

Adhesion; coating; polymer; molecular dynamics

## 1. Introduction

Due to its outstanding characteristics like high strength-to-weight ratio, machinability, workability, weldability and recyclability aluminium has been used in many structural and other applications [1]. However, under some conditions, aluminium and its alloys may remain unsuitable due to a lack of corrosion, erosion, fatigue or tribo-chemical wear resistance [2,3]. As per a report by National Association for Corrosion Engineers (NACE) International [4], it is appraised that the cost associated with overall corrosion is \$2500 billion worldwide, which is nearly 3.5% of the world GDP. It is predicted that by adapting current corrosion management strategies, savings somewhere between 15% and 35% of the cost of corrosion might be recovered, amounting to \$375–\$875 billion annually on a global level. By choosing proper material or corrosion control measures, the losses can be minimised to a larger extent [5]. Coatings are one type of preventative treatment that functions as a barrier between the surface and the surroundings. Anticorrosion coatings are metallic, non-metallic or organic. Organic coatings are widely used in industrial and structural applications as mostly polymers have methylene group ( $-\text{CH}_2-$ ) as the basic repeat unit which makes them hydrophobic which is one of the desirable characteristics of coating for metal protection. Polymeric coatings are therefore applied to metallic substrates as a thick barrier against corrosive species.

The analysis of interfacial interaction between two systems is an important subject for the growth and development of numerous engineering fields. Understanding the interfacial interaction is critical for investigating the miscibility and adhesion of distinct systems. Adhesion is a crucial factor for polymeric coatings as it defines the stability or bonding of

the polymeric coating to the metallic substrate. Thus, interfacial interaction or adhesion of polymer coatings on metallic or any kind of substrate can be quantified using the molecular dynamics simulations. Gee et al. [6] studied the adhesion of different fluoropolymers with 1,3,5-tri amino-2,4,6-trinitrobenzene (TATB). Two different TATB surfaces, viz. [1 0 0] and [0 0 1] were studied. It was revealed that the adhesion of TATB [1 0 0] was 45% more than TATB [0 0 1] as polymer spreads and diffuses more easily in TATB [1 0 0] due to larger surface area. Prathab et al. [7] investigated the influence of functional groups in the adsorption of PMMA onto different metal oxide surfaces like  $\text{Fe}_2\text{O}_3$ ,  $\text{Al}_2\text{O}_3$ ,  $\text{SiO}_2$  and  $\text{TiO}_2$ . The order of adhesion of PMMA with metallic substrates is as follows:  $\text{Fe}_2\text{O}_3 > \text{Al}_2\text{O}_3 > \text{SiO}_2 > \text{TiO}_2$ . It was observed that the intensity of the C–O–C bond increases in the order of metallic surfaces with less adherence to metal. Suárez et al. [8] studied the metal–polymer interaction between ferrous oxide and polyvinyl ester by varying the polymer chain length and found that adhesion is dependent on chain length also and increases as the chain length increases as atoms are capable of positioning themselves near to each other and hence non-bonded interaction enhances between polymer and metallic surfaces. The role of surface chemistry and surface roughness was studied by Quddus et al. [9] using MD simulations by studying the adhesion of oleic acid films to crystalline cellulose and found that planes with a larger surface area like [0 1 0] have better adhesion properties when compared to [1 0 0] and [1 1 0] planes. Anastassiou et al. [10] investigated the work of adhesion for pressure-sensitive adhesive (PSA) materials, viz. poly(*n*-butyl acrylate) and poly(*n*-butyl acrylate-co-acrylic acid) with substrates like silica ( $\alpha$ -quartz),  $\alpha$ -ferri-oxide and  $\alpha$ -ferrite in bulk and confined conditions. It was

also concluded that attaching acrylic acid to PSAs can enhance the adhesion at ambient temperature as a result of the existence of oxygen atoms in the acrylic acid. Yan et al. [11] employed MD simulations to investigate the interaction of poly-methyl methacrylate (PMMA) and polyvinyl acetate (PVA) with  $\alpha$ -quartz to examine the adsorption mechanism of both polymers with the substrate. It was revealed through the outputs of density profile and hydrogen bonding that the carbonyl group is a critical parameter for the interaction between two systems. Su et al. [12] investigated the adhesion of gypsum crystal on microfiltration membranes using experimental techniques and MD simulations. It was found experimentally that adhesion mass increases with increasing interaction energy between gypsum crystal and polymers, indicating that membrane chemistry like pore diameter is mostly responsible for adhesion mass. Xia et al. [13] studied the interfacial interaction between nanocellulose (NC) and PMMA using ordered cellulose nanocrystals (CNC) and amorphous cellulose (AC). It was found that the AC-PMMA interface has 50%–60% more adhesion energy as compared to CNC-PMMA due to the better dispersibility of AC in PMMA and greater hydrogen bonding. Liu et al. [14] explored the interfacial adhesion among the steel slag and asphalt both in dry and wet conditions. It was revealed that the reduction in adhesion due to moisture for steel slag was much lower than in limestone and quartz. It was because acidic minerals have weaker bonding whereas strong alkali has maximum. It is due to the strong electrostatic effect in strong alkalis. Heydari et al. [15] studied the impact of oxygen-containing groups on the adhesion between the polymer and metals using MD simulations. The adhesion of copolymers and terpolymers of maleic acid, vinyl acetate, and vinyl chloride with different configuration were studied with aluminium surface. The adhesion is greater in the tera-polymer containing the melic acid as compared to copolymer without melic acid with the same degree of polymerisation both at lower and higher temperatures. Peng et al. [16] investigated the role of silane-hydrolysate coupling medium on the interfacial interaction among bitumen and mineral aggregates using MD simulations. It was observed that the adhesion increases by using silane-hydrolysate both in wet and dry conditions. Also, the adhesion was greater in dry conditions when compared to wet conditions.

In the present study, the interaction of polyurethane (PU) and polytetrafluoroethylene (PTFE) on the aluminium oxide substrate have been analysed using MD simulations. The interaction of both polymers with the aluminium surface was studied at different temperatures. The key focus of the current investigation is to quantify the interaction between the PU and PTFE with the aluminium oxide substrate.

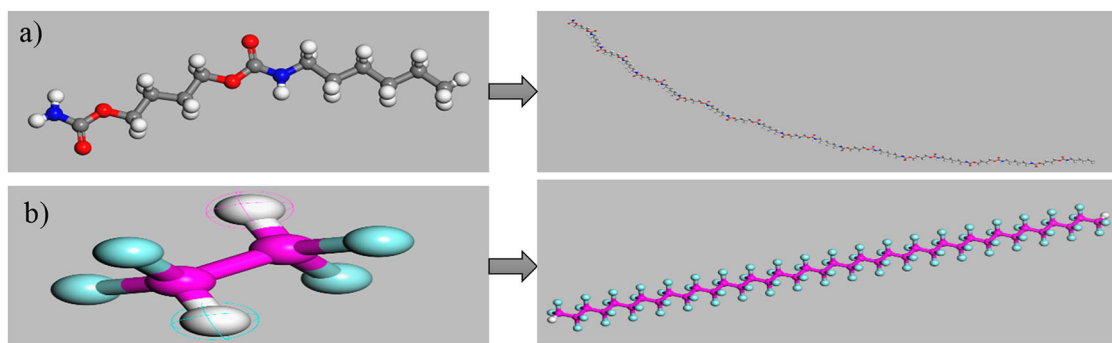
## 2. Materials and method

Polyurethanes (PU) are one of the most widely used polymeric coatings as it shows good adhesion with most metal substrates. Polyurethanes have characteristics like resistance to saltwater, excellent chemical resistance and thermal stability, resistance to UV rays, anti-fouling characteristics, excellent vibration and shock resistance, and can be used in a humid environment which makes them a potential candidate for corrosion

resistance [17]. Polytetrafluoroethylene (PTFE) is another polymer material used for coatings due to its extensive properties. The chemical inertness, hydrophobic nature, antifriction, non-stick and self-lubricating properties along with a high melting point of PTFE make it considerable for corrosion resistance [18–20]. Both the PU and PTFE are modelled in BIOVIA Materials Studio, 2017 with the degree of polymerisation equal to 20 and 10 as shown in Figure 1. COMPASS forcefield [21] is used in the present studies based on the previous studies by various researchers. Prathab et al. employed COMPASS forcefield to study the adsorption of poly-methyl methacrylate on the various metal oxide surfaces [7]. Wang et al. [22] also used COMPASS forcefield to study the adhesion of different acrylamide polymer flocculants with the aluminium oxide surface. Heydari et al. [15] also used COMPASS forcefield to study the influence of the oxygen-containing group in the adhesion of polymer films to the aluminium substrate.

Initially, a single chain of both PU and PTFE with degree of polymerisation 10 and 20, respectively, as shown in Figure 1 is geometrically optimised to refine the geometry of the chain using Smart algorithm until it reaches the specified convergence for energy and force which are  $1 \times 10^{-4}$  kcal/mol and  $5 \times 10^{-3}$  kcal/mol/Å [23]. Both the PU and PTFE are packed into the simulation box with starting density of 0.7 and 1.5 g/cm<sup>3</sup> in the three starting configurations. The polymers are packed in an amorphous cell with a confined layer to allow the system to create the lamellar system. The system is then geometrically optimised using Smart algorithm to get the minimum energy state of the packed system till the system reaches the specified energy and force convergence threshold. The configuration with minimum energy is selected for further analysis. Subsequently, the systems are equilibrated using an NPT ensemble for 1 ns at 298 K with pressure of 1 bar and time step of 1 fs. The thermostat and barostat were Anderson and Berendson, respectively. The NPT ensemble is chosen as polymer chains are packed at random densities. The final size of PU and PTFE cells was  $45.142 \times 45.142 \times 45.142$  Å and  $44.93 \times 44.93 \times 44.93$  Å. The aluminium oxide is then imported from the Materials Studio database and then cleaved [0 0 1] surface. The unit is then relaxed and geometrically optimised using Smart algorithm. The aluminium oxide unit cell is then extended to the superstructure of the size  $47.59 \times 47.59 \times 12.06$  Å.

The final metal–polymer system is made by using the layer module in Materials studio and the orientation of the bottom metal oxide layer is chosen and a vacuum of 100 Å is added after the polymer layer to break the periodicity of the system as shown in Figure 2 [9,24–26]. Subsequently, geometrically optimisation of the metal–polymer system is carried out by considering the metal layer as rigid [8,27]. The metal oxide layer is considered rigid as the metal geometry was already optimised as well as the structure may get distorted due to no covalent bond between aluminium and oxygen atoms of metal oxide. After geometry optimisation systems were annealed for two cycles with 50 heating ramps per cycle using NVT ensemble within the temperature range of 298 K–400 K for PU and 298 K–450 K for PTFE for 100,000 number of steps. The samples are annealed as there might be some local minima state for any sample after geometry optimisation. The different frames at the required temperature for



**Figure 1.** (Colour online) (a) Polyurethane. (b) Polytetrafluoroethylene. White = Hydrogen, Red = Oxygen, Blue = Nitrogen, Cyan = Fluorine, Grey(a) = Carbon, Magenta (b) = Carbon. Note: Magenta colour carbon atoms shows the backbone chain.

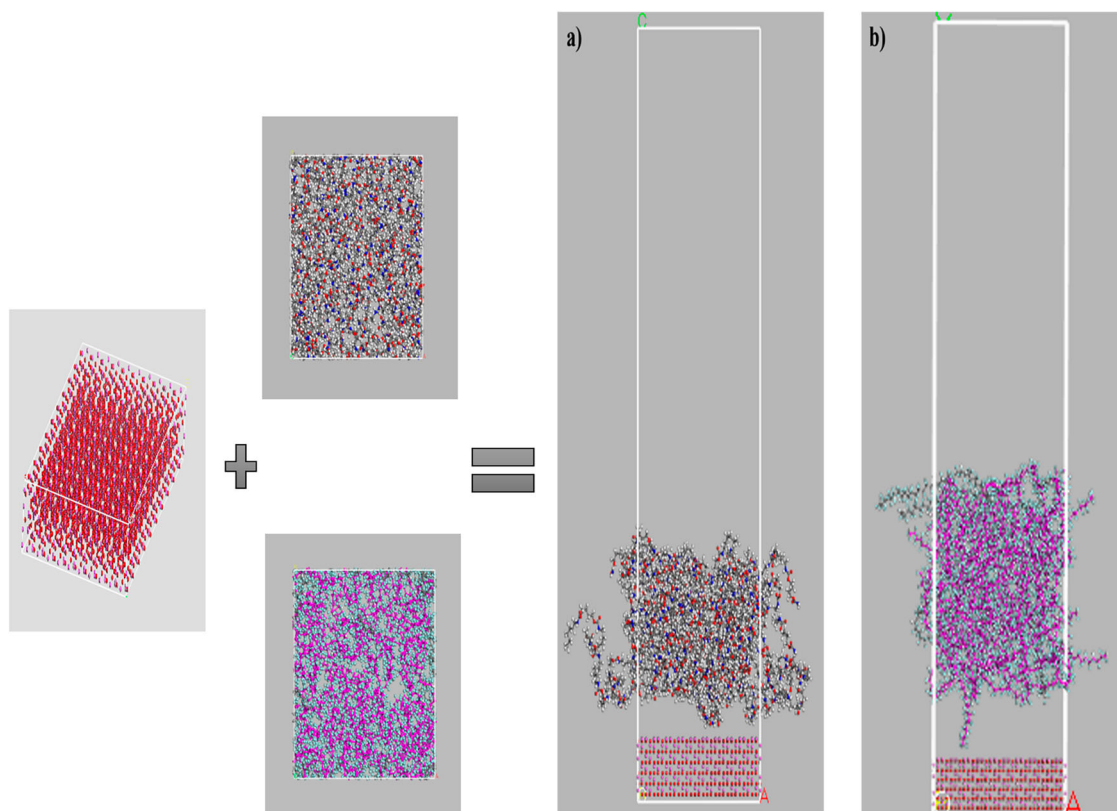
further dynamics are extracted from the cooling curve of annealing. This is done to get the samples at the particular temperature only. Further, the samples of both the PU/Al<sub>2</sub>O<sub>3</sub> and PTFE/Al<sub>2</sub>O<sub>3</sub> from annealing at 273.15, 285, 298 and 548 K are equilibrated for 1000 ps with a time step of 1fs. At NVT ensemble as shown in Figures 3 and 4. Although systems get equilibrated in small time but simulation is carried out for 1000 ps to avoid any instability in the samples. The same simulation is executed twice with same parameters to check any deviation in results. Although there are no such applications of both the polymers at such a high elevated temperature of 548 K, adhesion energy is calculated to predict the behaviour of interfacial adhesion of both polymers at very high temperatures. Finally, the energy for the whole metal–polymer, metal and polymer individually is calculated for further analysis purposes.

### 3. Results and discussion

Adhesion in two materials or surfaces can be predicted by the interaction energy between them. It is the energy needed to detach two different materials in vacuum and is due to non-bonded interaction between the two viz. van der Waals and electrostatic interactions. The more the negative value of interaction, the stronger will be the bonding between the two materials or more force will be required to separate both materials from each other. The following equation is used to calculate the interaction energy among the PU and PTFE and aluminium oxide surfaces.

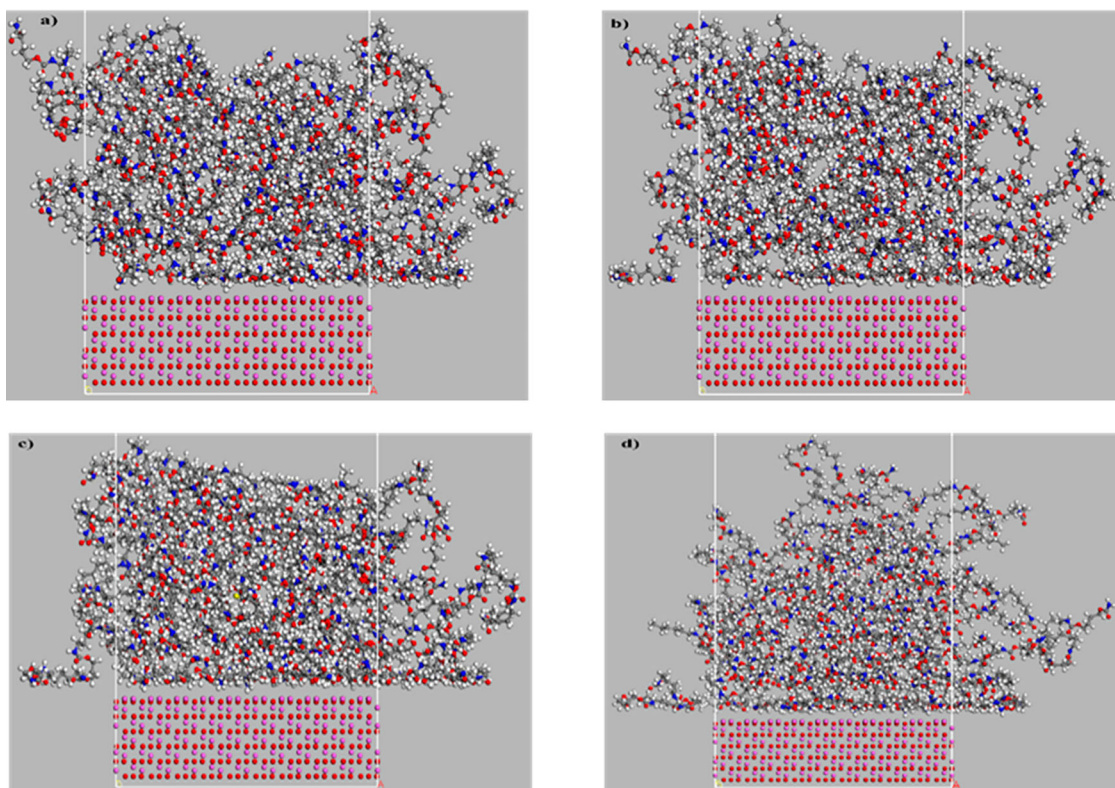
$$E_{\text{interaction}} = E_{\text{system}} - (E_{\text{metal}} + E_{\text{polymer}}) \quad (1)$$

$$E_{\text{adhesion}} = -(E_{\text{interaction}}) \quad (2)$$

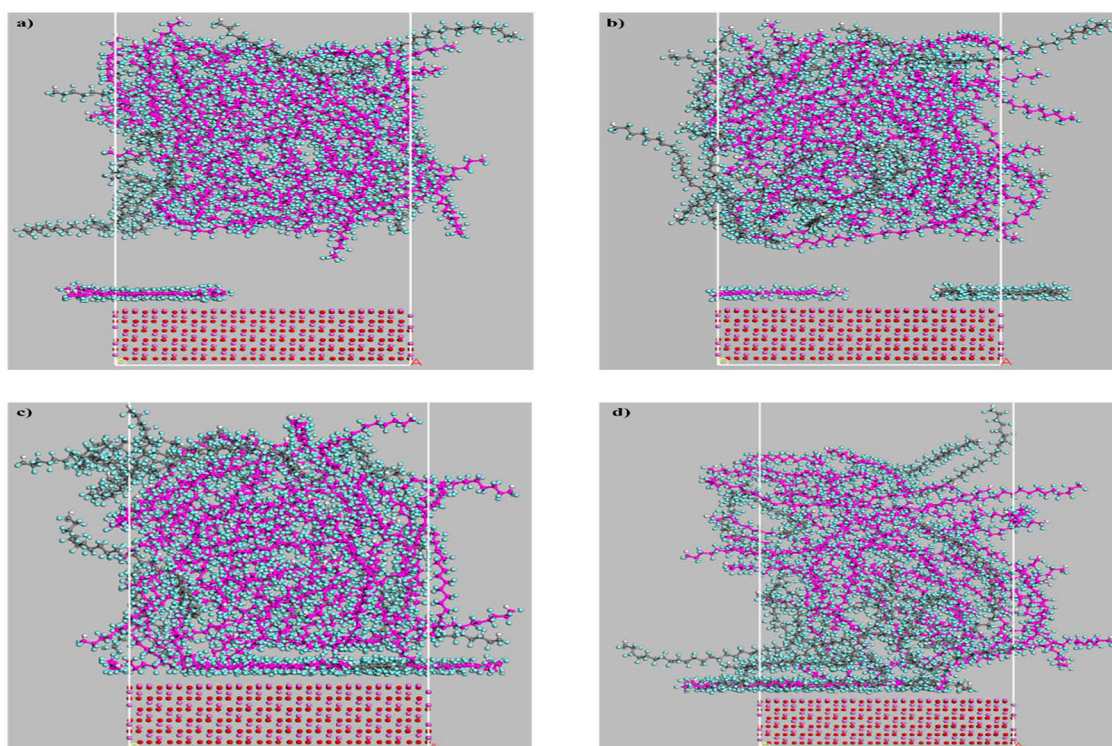


**Figure 2.** (Colour online) Initial metal–polymer system (a) PU–Al<sub>2</sub>O<sub>3</sub>, (b) PTFE–Al<sub>2</sub>O<sub>3</sub>.





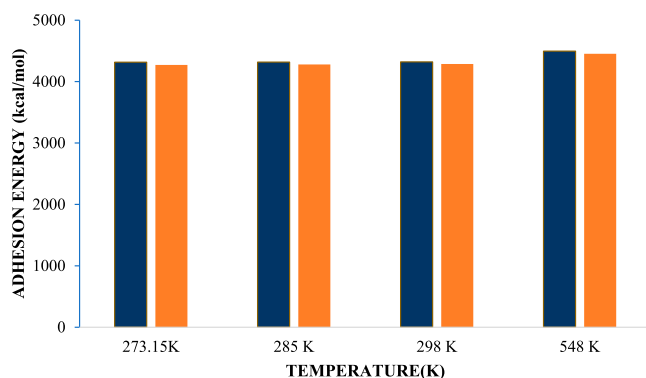
**Figure 3.** (Colour online) Final PU- $\text{Al}_2\text{O}_3$  system at (a) 273.15 K, (b) 285 K, (c) 298 K, (d) 548 K.



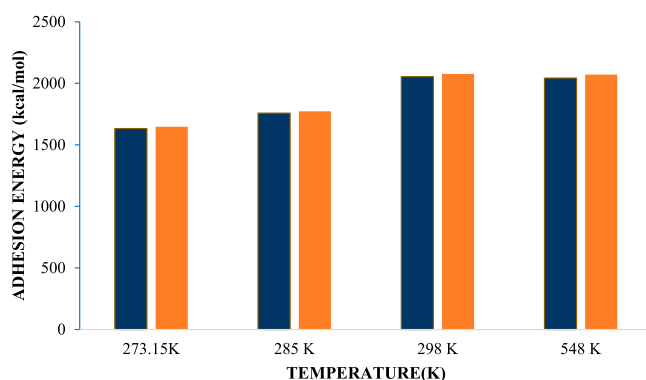
**Figure 4.** (Colour online) Final PTFE- $\text{Al}_2\text{O}_3$  system at (a) 273.15 K, (b) 285 K, (c) 298 K, (d) 548 K.

where  $E_{\text{interaction}}$  is the interfacial interaction energy,  $E_{\text{system}}$  is the total energy of the metal–polymer system,  $E_{\text{metal}}$  is the energy of the metal oxide layer and  $E_{\text{polymer}}$  is the energy of the polymer system. The interaction energy values for PU

and PTFE with almost same surface area with  $\text{Al}_2\text{O}_3$  at different temperatures are shown in Figures 5 and 6. The value of interaction energy at distinct temperatures is tabulated in Table 1.



**Figure 5.** (Colour online) Value of adhesion energy for PU at different temperatures.



**Figure 6.** (Colour online) Value of adhesion energy for PTFE at different temperatures.

The negative value of interaction energy gives the adhesion or bonding energy. It was specified that the positive value of adhesion energy can signify certain interactions of hydrogen bonds or electrostatic interactions among atoms of systems [28]. As the temperature increases the adhesion energy of both polymers increases in the range from 273.15 K to 298 K. For the polyurethane, the percentage change of energy with temperature is small which depicts its stability with temperature. For PTFE the percentage change with temperature is more when compared to PU. However, for PTFE at 548 K the adhesion energy is less when compared to 298 K which may be due to the factors like the orientation of polymeric chains which has a good agreement with the result obtained by Heydari et al. [15] for interaction energy between copolymer of vinyl acetate and vinyl chloride and terpolymer of vinyl acetate, vinyl chloride and maleic acid with same  $\text{Al}_2\text{O}_3$  substrate at 298 and 548 K that interaction energy was little lesser at 548 K when compared to 298 K. The gain in the adhesion energy with the rise in the temperature is possibly

due to increased mobility of molecular chains which is a good agreement with Gao et al. [29] that adhesion energy increase with the increase in temperature. The repeatability of the results can be seen from Table 1.

#### 4. Conclusions and future scope

The present work quantifies the interfacial adhesion among the aluminium oxide substrate and PU/PTFE coatings using molecular dynamics simulations. The major conclusions drawn from the present study are as follows:

- The rise in the temperature resulted in the gain in the adhesion of both polymers with the metal surface. However, there is a slight decrease in the adhesion of PTFE with metal oxide at a very high temperature.
- The possible reason for the increase in the adhesion between polymer and metal is due to an increase in the flexibility of the polymer chains with temperature rise.
- The change in interaction energy for PU in the range of 273.15–298 K is relatively less when compared with percentage change for PTFE in the same range.
- The value for adhesion energy for PU was much greater than PTFE at all investigated temperatures.

The present study gives a good insight into the adhesion of PU/PTFE with an aluminium surface and can be further extended in finding the adhesion of different polymers, copolymers, composites films and paints oils with other surfaces. Adhesion is an important phenomenon between the two different systems and thus this study can give an approach to analysing the interaction of different systems at interfaces.

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#### Disclosure statement

No potential conflict of interest was reported by the author(s).

#### Data availability statement

The raw/processed data required to reproduce these findings cannot be shared at this time due to legal or ethical reasons. The data will be made available on request.

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**Table 1.** Interaction energy values for PU/PTFE- $\text{Al}_2\text{O}_3$  at different temperatures.

Temperature	$E_{\text{int-PU}}$ (kcal/mol)		% Error (PU)	$E_{\text{interaction-PTFE}}$ (kcal/mol)		%Error (PTFE)
	Iteration 1	Iteration 2		Iteration 1	Iteration 2	
273.15 K	−4314.758	−4271.648	0.99	−1632.299	−1647.132	0.90
285 K	−4316.996	−4279.063	0.87	−1757.675	−1772.332	0.83
298 K	−4319.366	−4286.487	0.76	−2054.196	−2076.758	1.09
548 K	−4494.936	−4452.418	0.94	−2042.551	−2071.315	1.4

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