Comparative study of graphene-polypyrrole and borophene-polypyrrole composites: molecular dynamics modeling approach

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A R T I C L E I N F O	A B S T R A C T
	In the search for the solution to energy storage problems, this study investigates the interfacial energy interaction and temperature stability of the composites made of polypyrrole-graphene-borophene (PPy-Gr-Bon) by using molecular dynamics simulations. From the calculated thermodynamics and interfacial energies of the system, comparisons between the ternary and the binary-binary systems were made. The materials in the entity show a good degree of temperature stability to a dynamic process at 300, 350, 400, and 450 K. Moreso, at 300 K, the interaction energy of PPy-Gr, PPy-Bon, and PPy-Gr-Bon are: $-5.621e^3$ kcal/mol, $-26.094e^3$ kcal/mol, and $-28.206e^3$ kcal/mol respectively. The temperature stability of the systems is in the order of: PPy-Gr-Bon > PPy-Bon > PPy-Gr. The effect of temperature on the interaction energy of the systems was also investigated. The ternary system showed higher stability as the temperature increased. In addition, the radial distribution function computed for the three systems revealed that there is a strong, but non-chemical bonding interaction between PPy-Gr-Bon, Bon-PPy, and Gr-PPy. By considering the excellent mechanical properties of PPy-Gr-Bon and the already established high electrical conductivity and chemical stability of Gr, Bon and PPy, their composite is therefore suggested to be considered for the manufacturing of electrochemical electrodes.

1. Introduction

The intermittent nature of renewable energy resources, such as: solar and wind energy gives rise to the urgent need for electrochemical energy storage devices (EEDS) (POIZOT *et al.*, 2011). Fossil fuel menaces and its negative environmental impact can be reduced by meaningfully engaging the use of EEDS in aerospace, transportation, and grid power industries. However, as useful alternatives as EEDS are, there are lots of challenges confronting their reliability, dependability, and sustainability. One of the contributing factors to the problems of EEDS, is the material responsible for the manufacturing of electrodes. Electrochemical storage electrode (ESE), determines the power and energy density of the storage device. In addition, the safety of electrochemical devices is a function of the electrode. For these

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reasons, new materials that will substitute the current electrodes, cannot be overemphasized (Sun *et al.*, 2013; Y. Zhang *et al.*, 2019). A suitable electrode can be manufactured by the use of polymer-composite (Xu *et al.*, 2020).

Graphene is a 2D allotrope of carbon with exceptional properties, especially for energy storage (Ji *et al.*, 2016). The properties of graphene for multi-application have been investigated by several researchers (Abergel *et al.*, 2010; Fan *et al.*, 2015). The extensive study of graphene and its properties is as a result of its excellent electrical conductivity, good chemical and thermal stabilities, flexibility, and mechanical strength. Flexible-bendable graphene electrode was produced by (Gwon *et al.*, 2011). The possibility of this emerged due to the advantage of graphene mechanical flexibility and superior electrical conductivity of graphene. An electronic gas-based sensor was fabricated from graphene oxide by (Bo *et al.*, 2014), by employing caffeic acid as a reducing agent. The large surface area of graphene is another good property which makes it a good candidate for supercapacitor energy storage. Amongst the various factors, such as: ultra-high surface area, good conductor of electricity, thermal and chemical stabilities, high tensile strength and the excellent flexibility properties of graphene, merit or qualify the magic material to be classified as suitable for energy storage and electronics purposes (bin MohdáYusoff, 2015; Dai *et al.*, 2014).

The stability of the covalently bonded molecular network of carbon is similar to that of boron; therefore, boron is analogous to carbon. Borophene is a recent 2D material, having a single layer of boron sheet. This single layer of boron sheet has been produced from the synthesis of boron on substrates, such as: copper, (Cu(111)), aluminum, (Al(111)), gold, (Au(111)), and silver (Ag(111)) (Abadi *et al.*, 2020; Li *et al.*, 2018). Large surface area, very high electrical conductivity, flexibility, and large electron mobility strength are some very desirable advantages of borophene. The possibility of making a transparent electrode from boron was investigated and suggested by (Adamska *et al.*, 2018). In the theoretical investigation of borophene as energy storage material, Folorunso et al., (Folorunso *et al.*, 2020b) reported that borophene is a good candidate material for lithium-ion batteries due to its high specific capacity. Another advantage of borophene is in the way its properties can be easily controlled in order to obtain other materials which may be useful for different applications (bin MohdáYusoff, 2015).

Polymers have the tendency to retain their properties when two dimensional (2D) materials are added to them. In fact, it has been shown that polymers exude better properties when composited with 2D-materials (Li *et al.*, 2017; Z. Yuan *et al.*, 2016). Polypyrrole and polyaniline have been demonstrated as good materials for microactuators devices based on their ability to change volume when undergoing electrochemical doping and de-doping processes (Jager *et al.*, 1999). Among the various types of conducting polymers, polypyrrole is a very promising electrochemical energy storage material, due to its environmental-benign, chemical stability, low cost, simple synthetic methods, high energy storage capacity, good electrical conductivity, thermal conductivity, and mechanical stability (Kim *et al.*, 2016; Stejskal *et al.*, 2018).

Molecular dynamics simulation is a modeling simulation approach used to study particle dynamics and inter-atomic force models (Karataraki *et al.*, 2019; Mazo *et al.*, 2019). Molecular dynamics is concerned with simulations of a molecule's physical motions in such a way that these molecules are treated as computational particles (Sui *et al.*, 2015). The equilibrium and nonequilibrium of the physical phenomena can be simulated and analyzed by molecular dynamics. Some empirical or experimentally derived potential functions (force fields) are usually engaged to monitor the interactions between the particles. Polymers and their composites require extensive investigations through modeling and simulations and this will reduce experimentation cost and improve the accuracy of expected results (Folorunso *et al.*, 2019). Density function theory (DFT) can also be used to predict the properties of materials (Hanindriyo *et al.*, 2020). DFT can predict the electronic, structural, and magnetic properties of material. However, molecular dynamics is used to investigate the dynamic properties of materials using Newton equation (Ghafelehbashi *et al.*, 2020; Tanzifi *et al.*, 2020). Composite is the

combination of different materials in order to modify their various properties for desired applications. For polypyrrole to effectively function as a supercapacitor or battery electrode, other materials must be added to it. A large attendant of researchers has investigated the composite of polymer and 2D-materials for energy storage (FOLORUNSO *et al.*, 2020a; MA *et al.*, 2016).

The theoretical synthesis of graphene-polypyrrole was performed by (JIA *et al.*, 2013) and the interfacial behaviors of the graphene-polypyrrole were computed by using the molecular dynamics simulations. Dewapriya et al. (2019) used a molecular dynamics simulation approach to investigate the energy dissipation mechanisms of graphene loaded polyethylene. Petucci et al. (2013) studied the dynamic properties of hydrogen on graphene using molecular dynamics in conjunction with AIREBO potential. Picaud et al. (2005) investigated the electrical conductivity of highly concentrated liquid electrolytes by using the molecular dynamics simulations. The combination of Monte Carlo simulation and molecular dynamics has been used to predict the electrical conductivity of carbon, silicon, germanium, and tin (TSUBOI *et al.*, 2006). The diffusion coefficient or transport behaviors of water content and ions in clay has been investigated by Greathouse et al. (2016), by using molecular dynamics simulations. The characteristics properties of the composite of polymer (epoxy) and boron-nitride in the presence of an organic functional group was investigated by Li et al. (2019). Graphene and biological substance composites have been experimentally produced, dynamically simulated, and reported by Macwan et al. (2017). Biosensors can be manufactured from the composite of graphene-proteins due to the high conductivity and surface area of graphene. The first molecular dynamics simulations on polypyrrole-water interaction were conducted by Lopez-Cascales et al. (2003). The density, distribution of atoms, and thickness of the polypyrrole-water were the parameters computed.

This study focuses on the temperature distribution and the interaction energies of binaries systems of borophene-polypyrrole, graphene-polypyrrole and a ternary system of borophene-graphene-polypyrrole by using molecular dynamics simulations method in conjunction with the Lennard-Jones (Lj) and the Tersoff potentials. The study observed that borophene has better interaction with polypyrrole than graphene and it shows excellent thermal stability with the polymer. The ternary system gives a slight energy interaction difference than the binary system of borophene-graphene. However, the binary system of graphene-polypyrrole shows high energy interaction disparity from the ternary system. Moreover, the ternary system experienced higher temperature stability than the binary-binary system. Furthermore, this study suggests the ternary system of borophene-graphene-polypyrrole for electrochemical energy electrode due to the composite thermal energy stability, low mass degradation, and very high energy interaction.

2. Materials and Methods

The calculations in this study were performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package (PLIMPTON, 1993) in conjunction with hybrid potentials. The input data files of the molecular structures of the systems were developed and generated using Materials Studio (Accelrys, San Diego, CA, US) (ACCELRYS, 2010), and then imported into LAMMPS code. The open visualization tool (OVITO) software (STUKOWSKI, 2009), was used to visualize the trajectories of the molecular dynamics. For the molecular dynamic simulations using the LAMMPS, the hybrid potential consisting of Lennard-Jones and Tersoff, were the potentials engaged to investigate the interaction of the atoms of polypyrrole with borophene and graphene. The force of attraction and repulsion of the particles defined by Eq. 1, is called the Lennard-Jones (ℵ) potential (MCDONALD *et al.*, 1967).

$$\aleph(\lambda_{jk}) = \frac{\epsilon_{jk}}{0.25}\left(\left(\sigma_{jk}\lambda_{jk}^{-1}\right)^{12} + \left(\sigma_{jk}\lambda_{jk}^{-1}\right)^{6}\right) \tag{1}$$

In here, ϵ is the potential well depth, σ is the diameter at collision, the label j and k are the atoms in the model, and λ is the particles separating distance. The ℵ-potential parameters used in this study are itemized in Table 1.

Table 1. ℵ-potential parameters used in this study

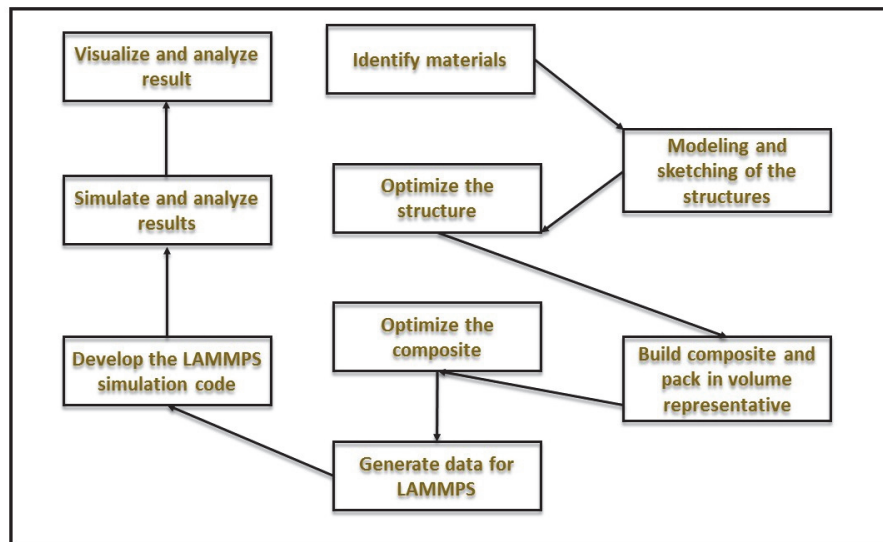| S/N	Model	ϵ_{ij} (eV)	σ_{ij} (Ang)	References
1	C – N	0.08700	7.861	(VEKEMAN et al., 2018)
2	C – H	0.34080	1.091	(AU, 2012)
3	C – C	0.00284	3.400	(AU, 2012)
4	H – H	0.00150	2.650	(AU, 2012)
5	N – N	0.00710	3.680	(EVANS, 1977)
6	B – B	0.09490	3.453	(HILDER et al., 2010)
6	H – N	0.03800	2.450	(ACCELRYS, 2010)

The Tersoff-potential presented by (KINACI *et al.*, 2012), was used to provide the interaction between the boron, nitrogen, and carbon. The computational procedures are explained in the block diagram of Fig. 1.

2.1. The Simulation models

In this study, two binary systems, consisting of graphene loaded polypyrrole, borophene loaded polypyrrole, and their ternary system, were investigated by using molecular dynamic simulation. The matrix is the polypyrrole, while graphene and borophene were used as the reinforcement. A single layer of graphene having a supercell of $6 \times 6 \times 1$ was packed into a simulation cell having dimensional set of $24 \times 24 \times 24$ Å^3, and containing 624 atoms. The dimension of the borophene is $3 \times 3 \times 1$ supercell and the simulation cell contain 624 atoms of boron with dimension $24.1 \times 24.1 \times 24.1$ Å^3. The single chain of the polypyrrole considered in this study, is as shown in Table 2. The 3D molecular structure of the polypyrrole, was constructed with $26.2 \times 26.2 \times 26.2$ Å^3 dimension. Convergence of results is obtainable with a 122 unit of monomers (Z. YUAN *et al.*, 2016). The matrix contains 1220 atoms.

Table 2. A single chain polymer parameter

S/N	Polymer	Weight	Stoichiometry	Monomer
1	PPy	976 g/mol	$C_{60}H_{45}N_{15}$	122

Fig. 1. Block diagram of the computational procedures.

2.2. The Simulation processes

In this study, the Newton motion equation of the systems is solved by using the Verlet algorithm (VERLET, 1967). The Verlet algorithm was used to measure the velocity of each particle with respect to time change. The systems' temperatures were controlled and maintained by Langevin (SCHNEIDER *et al.*,

1978). Periodic boundary conditions were used in the transverse and longitudinal directions. In addition, the interaction is described by the hybrid potentials of Tersoff, and Lennard-Jones.

Before carrying out the equilibration of the structures and their composites, minimization was executed by using the minimize command in LAMMPS: stopping tolerance for energy and force, were $1.0e^5$, and $1.0e^5$, maximum iterations of the minimizer and the number of force-energy evaluations were $1.0e^5$ and $1.0e^6$ respectively. The minimization was used to achieve a sensible distribution state. To relax the systems, the unit cells were equilibrated for 500 ps with a small time step of 0.01 fs under NVT (constant moles (N), volume (V), and temperature (T)) ensemble at a temperature of 300 K. Afterward, a NPT (constant moles (N), pressure (P), and temperature (T)) ensemble dynamic system was performed at 300 K for 5 ns with a time step of 0.01 fs. The run step was set at 1000, so as to obtain data for subsequent analysis and calculations of the properties of the binary and ternary systems of hybrid graphene-borophene loaded polypyrrole. To consider the effect of temperature on the interaction energy of the systems, a temperature range of 300 - 450 K were considered. The composite of the three materials is as shown in the cell box of Fig. 2.
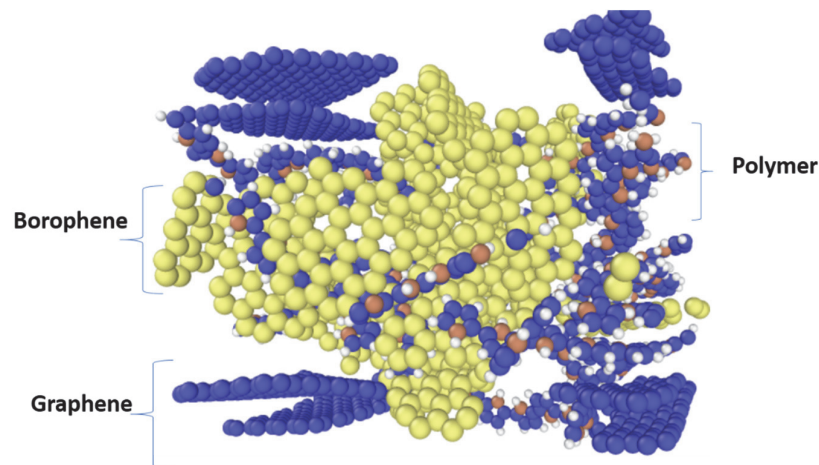

Fig. 2. Hybrid of Gr-Bon loaded PPy.

3. Results and Discussion

The thermodynamics and the interfacial study of the ternary and binary systems of graphene-borophene-polypyrrole have been studied, using molecular dynamics simulations. The comparative study showed that the binary system of borophene-polypyrrole has better energy interaction and low mass loss degradation than the binary system of graphene-polypyrrole. Further potential improvement in the structural behaviors and thermodynamics properties were recorded for the ternary system of the materials. In this section, the temperature analysis, and the interaction energies of ternary/binary systems of polypyrrole, graphene, and borophene have been discussed, *viz*: the molecular thermodynamics simulations results.

3.1. Temperature and equilibrium analysis of the system

The temperature evolution (Φ) curves for the PPy-Gr-Bon, PPy-Gr, and PPy-Bon composites were investigated and displayed in Fig. 3(a-c). The composite systems of graphene, borophene, and polypyrrole, show high stability at the given temperatures. The fluctuation in the temperature was as a result of the random movement of the particles, nonetheless, the exhibited temperature differences can be assumed negligible. At 300 K, the percentage of oscillation within the specified 5 ns for Bon, Gr, and PPy, are: 22.62%, 24.41%, and 18.7%, while the PPy-Gr, PPy-Bon, PPy-Gr-Bon composites gave temperature difference of 14.55%, 13.39%, and 12.92%, respectively. The temperature stability of the system is in the order of: PPy-Gr-Bon > PPy-Bon > PPy-Gr. From Fig. 4, it can be seen that the potential energy of the individual system remains almost equal and repeatedly oscillates within the specified time.

In addition, the systems converged at the stipulated time. Therefore, the temperature and the energy evolution of the systems, evident the thermodynamic stability of the composites.

From the calculated results, it was observed that the incorporation of graphene and borophene into the polymer improves the thermal stability of the ternary system. Among others, the thermal stability of graphene and borophene can be attributed to their relative low phonon frequencies, which is inversely proportional to entropy, thus, leading to their high stability (KINLOCH *et al.*, 2018; PENG *et al.*, 2017). The negative impacts of temperature on the electrochemical electrodes, such as cracking and fracture, safety, charge degradation, and lifespan, have been the problems confronting the development and manufacturing of high power and energy density electrochemical devices. In a way, if the problem of temperature can be minimized in electrochemical energy storage devices, then energy storage technology will be more matured (LENG *et al.*, 2015; MALEKI *et al.*, 2001).

Moreover, the constant moles (N), volume (V), and energy (E) command were used to obtain the temperature evolutions of the systems. The thermodynamics temperature curves of the systems are given in Fig. 5. As shown in Fig. 5, PPy-Gr-Bon exhibits very low temperature rise when compared to Gr-PPy and Bon-PPy. In order to have a further comparison, it can be seen that Bon-PPy exhibits lower temperature rise than Gr-PPy. This effect is explained in terms of mass loss/degradation as investigated by (RAHMANI *et al.*, 2017). Therefore, PPy-Gr-Bon composite with the lowest temperature rise will experience the lowest mass loss/degradation. This behavior is desirable for electrode and energy harvesting materials.
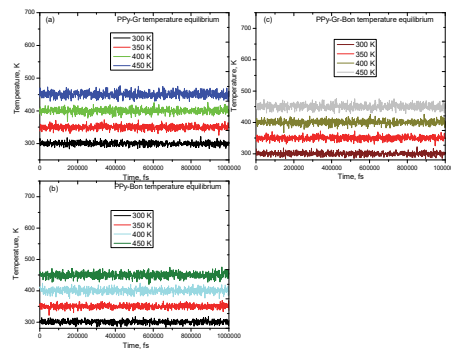

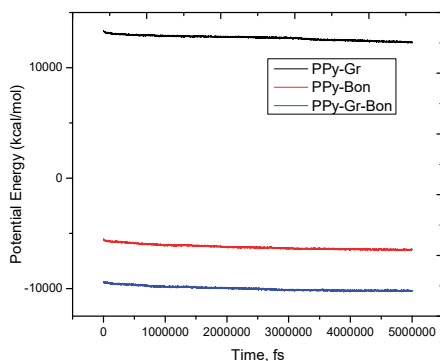**Fig. 3.** (a) Φ curve of PPy-Gr (b) Φ curve of PPy-Bon and (c) Φ curve of PPy-Gr-Bon

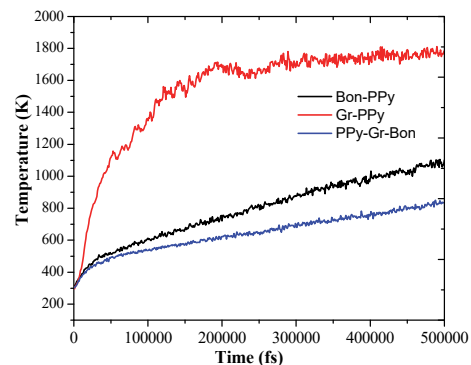**Fig. 4.** Energy evolution curves of PPy-Gr, PPy-Bon, and PPy-Gr-Bon

Fig. 5. Φ evolution curve for the Bon-PPy, Gr-PPy, and PPy-Gr-Bon composites

3.2. Analysis of the interaction energy

In order to establish if there was any interaction between the 2D-materials and the polymer, Eq. 2, is defined, thus:

$$\gamma_{int} = \gamma_{total} + \left(-\sum \gamma_{ind}\right) \tag{2}$$

where γ_{int} is the total interaction energy, γ_{total} ($\gamma_{Bon+PPy}, \gamma_{Gr+PPy}, \gamma_{Bon+Gr+PPy}$), is the total energy of the composites, and γ_{ind} ($\gamma_{Bon}, \gamma_{Gr}$, and γ_{PPy}), is the energy of the individual material. The γ_{total} in Eq. 2, is the total energy of the system. The interactions between the polypyrrole and the 2D-materials are due to van der waals (γ_{vdW}), π - π interactions $\gamma_{\pi-\pi}$ and electrostatic (γ_{Coul}) energies (JIA $et\ al.$, 2013), as shown in Eq. 3 (ZAMINPAYMA, 2014).

$$\gamma_{sys} = \gamma_{Coul} + \gamma_{vdW} + \gamma_{\pi-\pi} \tag{3}$$

At the specified molecular weights (Mw) of all the individual material, the thermodynamic study of the binaries and ternary systems of the composites, were carried out. Table 3, is the results of the interactions and the energies of the systems at 300 K.

Table 3. The systems and their interaction energies

S/N	Materials	γ_{ind} (kcal/mol)e^3	γ_{total} (kcal/mol)e^3	γ_{int} (kcal/mol)e^3
1	PPy	21.058		
2	Gr	-1.085		
3	Bon	0.450		
4	PPy-Gr		14.352	-5.621
5	PPy-Bon		-4.586	-26.094
6	PPy-Gr-Bon		-7.783	-28.206

The compatibility of the polypyrrole with graphene and borophene, is further displayed in Table 3. A $-5.621e^3$ kcal/mol interaction energy was calculated for the PPy-Gr composite while PPy-Bon has $-26.094e^3$ kcal/mol. The interaction energy of the borophene with polypyrrole is significantly higher than that of graphene with polypyrrole. Both 2D materials have strong interactions with the polymer, however, borophene shows higher energy interaction with polypyrrole. Moreover, a total energy interaction of $-28.206e^3$ kcal/mol was calculated for the composite of the hybrid graphene, borophene loaded polypyrrole. From literature (JIA $et\ al.$, 2013; OYINBO $et\ al.$, 2020), the energy of a system is expected to be negative before a conclusion can be drawn on whether there is attraction or repulsion between the particles. The more negative the interaction, the greater their interaction energy. The negative values of the interaction energies of these composites revealed the fact that the 2D materials have good interactions with the polymer and during the dynamic process, they produced heat.
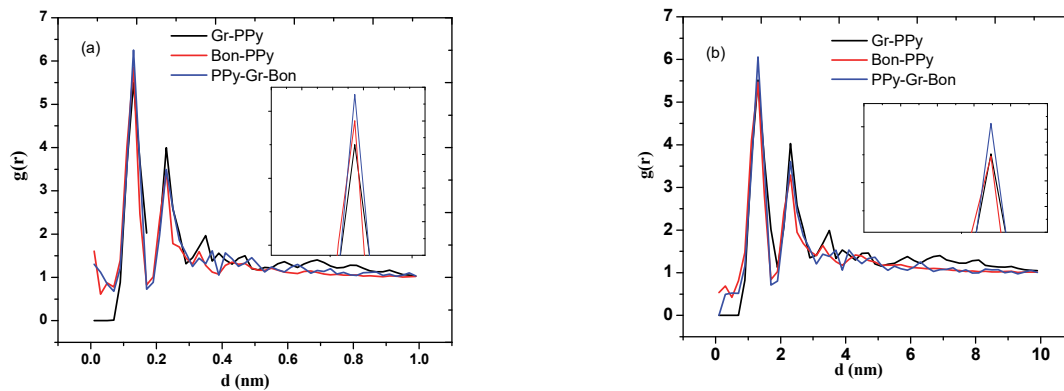

Fig. 6. Radial distribution function of the systems at (a) 0.2 ns (b) 0.5 ns.

The radial distribution function (RDFg(r)) in Fig. 6, provides information that is related to the atomic density of each of the systems at 0.2 ns and 0.5 ns. The g(r) curves show the peaks of the three systems. The maximum peaks computed for the composites are: 6.26, 5.86, and 5.41, when d equals 0.13 nm, 0.128 nm, and 0.12 nm respectively, corresponding to PPy-Gr-Bon, Bon-PPy, and Gr-PPy. The peaks of these systems also explain the changes in the structures and the interaction energies of the composites. Evidently, there exist strong non-chemical bonds (van der Waals) interaction in the PPy-Gr-Bon composites than Bon-PPy and Gr-PPy. Therefore, the justification to the interaction energies of these three systems is hereby justified by the peaks of systems (JIA *et al.*, 2013; LI *et al.*, 2019).

3.3. Temperature effects on the interaction energy

The optimal processing temperature is determined by considering the effects of dependence of binding energy on the temperature capability of the composite. In effect, to properly saturate additives into the polymer matrix, a certain temperature threshold must be known. Processing the composite at higher temperature greater than the threshold temperature, the composite may lose its thermal properties. The temperature is inversely proportional to the system aspect ratio (OYINBO *et al.*, 2020). When the aspect ratio of the system decreases, binding energy decreases. This means that a low aspect ratio is associated with poor electrical and mechanical properties; low binding energy binding will result in low composite integrity. As nanomaterials can improve and tune the properties of other materials, so also it can cause damage to them. The study of the temperature effect on the binding energy of the system is very important, so as to obtain the precise process temperature of the system. Moreso, for commercial applications of composites materials, their thermal stability investigation, is very crucial.

Since the maximum temperature necessary to achieve stability in polypyrrole is between 423 - 473 K (BISWAS *et al.*, 1994; MAVINAKULI *et al.*, 2010), then, 300, 350, 400, and 450 K were considered to describe the effect of temperature on the interaction of the composites. Table 4 shows the variation in the energies of the binaries and the ternary systems with respect to temperature. In Fig. 7, the temperature effect on the PPy-Bon and PPy-Gr-Bon, is displayed. As it is shown in Fig. 7, the interaction energy of the ternary system of PPy-Gr-Bon is stronger than that of PPy-Bon at 300 and 350 K. However, as the temperature keeps increasing, the interaction energy of PPy-Bon shows linear relationship with the temperature, while the interaction energy of the ternary system of PPy-Gr-Bon decreased at temperature above 350 K and tends to be stable as the temperature increases. The high interaction energy of the two systems is an evidence of improvement in the mechanical properties of the composites (SHI *et al.*, 2020). Also, the stability of the ternary system means that the mass loss/degradation of the composite will be reduced as the temperature increases (RAHMANI *et al.*, 2017). This behavior is desirable for electrode and energy harvesting materials. Moreover, Fig. 8 shows the comparison of temperature effects on the binary systems of PPy-Gr and PPy-Bon. It is observed from **Fig. 8** that the interaction energy of the binaries systems increases as the temperature increases, however, there is disparity in the interaction energy of PPy-Gr and PPy-Bon. The interaction energy of the PPy-Gr composite attained 400 K before it started decreasing. These results are in agreement with the investigations of several authors (VILLAR-RODIL *et al.*, 2009; J. YUAN *et al.*, 2015; Z. ZHANG *et al.*, 2017).

Table 4. Temperature effect on energy

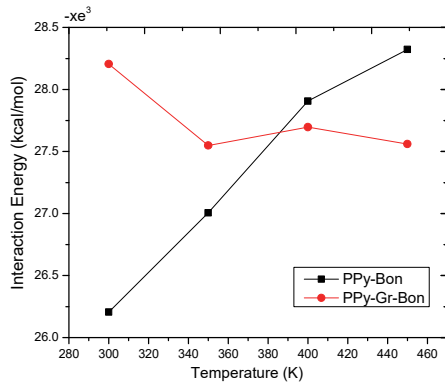| S/N	Materials	γ_{ind} (300k) (kcal/mol)e^3	γ_{ind} (350 K) (kcal/mol)e^3	γ_{ind} (400 K) (kcal/mol)e^3	γ_{ind} (450 K) (kcal/mol)e^3
1	PPy	21.058	21.267	21.632	21.989
2	Gr	-1.085	-0.822	-0.642	-0.457
3	Bon	0.450	0.626	0.854	1.049
4	PPy-Gr	14.352	14.710	15.153	15.740
5	PPy-Bon	-4.586	-5.113	-5.420	-5.285
6	PPy-Gr-Bon	-7.783	-6.477	-5.852	-4.987

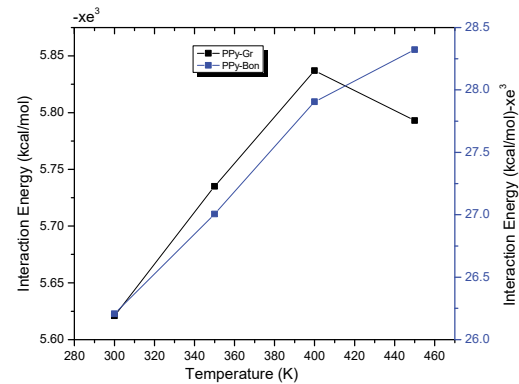**Fig. 7**. Effect of temperature on the interaction energy of PPy-Bon and PPy-Bon-Gr-Bon

Fig. 8. Effect of temperature on the interaction energy of PPy-Gr and PPy-Bon

4. Conclusion

In conclusion, molecular dynamics simulations have been employed to investigate the interactions of the atoms of borophene, graphene and polypyrrole. Thermodynamically, the composites of PPy-Gr-Bon, PPy-Gr, and PPy-Bon are stable under temperature excitation. Firstly, the study observed that borophene has a higher affinity with conjugated polypyrrole than graphene. Secondly, during the dynamic process, temperature differences of 14.5%, 13.39%, and 12.92% were observed for PPy-Gr, PPy-Bon, and PPy-Gr-Bon, respectively. Thirdly, the temperature effect on the interaction energy of the systems revealed the thermodynamics behaviours of the systems, whereby, PPy-Gr-Bon composite maintains almost constant interaction energy as the temperature increases. Moreover, the interaction energy of the binary systems shows linear relationship within the specified temperature. Nevertheless, at temperature beyond 400 K, interaction energy of the composite of PPy-Gr sharply reduced. The PPy-Gr-Bon hybrid composite would have lower mass loss/degradation than the PPy-Gr and PPy-Bon composites. Furthermore, the overall interaction energy of the ternary system, i.e., PPy-Gr-Bon composite is higher than the PPy-Gr composite by 79.30%, and PPy-Bon by 0.01%. It can be inferred from these results that borophene and graphene are good materials for the modification of the properties of polypyrrole for the manufacturing of electrochemical electrodes due to its thermal stability, low mass degradation, and very high interaction energy. Consequently, it is envisaged that the hybrid of graphene-borophene-polypyrrole is very promising for salvaging the inherent problems associated with electrochemical energy storage.

Acknowledgment

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