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**Submission date:** 17-Jan-2022 02:10PM (UTC+0700)

**Submission ID:** 1742874985

**File name:** Artikel-15.pdf (1.28M)

**Word count:** 5243

**Character count:** 24276

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To cite this article: N A Sasongko *et al* 2020 *J. Phys.: Conf. Ser.* **1524** 012084

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# Understanding the interaction of polysulfone with urea and creatinine at the molecular level and its application for hemodialysis membrane

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**Abstract.** The formation of polysulfone and its interaction with urea and creatinine have been evaluated at the density functional theory (DFT) level (B3LYP/6-31G\*\*) to study the transport phenomena in hemodialysis membrane at a molecular level. The energy interaction of PSf-creatinine and PSf-urea complexes are -3.87 kcal/mol and -6.31 kcal/mol, respectively; which were classified in weak hydrogen bond interaction. Furthermore, the size of the urea is smaller than creatinine by 5.6 and 3.2 Å, respectively. All data presented that urea has a stronger interaction with PSf than creatinine that indicated urea easier to transport in the PSf membrane than creatinine during the hemodialysis process.

## 1. Introduction

The people who suffer the Chronic kidney disease (CKD) significantly increased in every year in the world. The several treatments to help the patients are peritoneal dialysis, kidney transplantation, and hemodialysis. Whereas, hemodialysis is the common treatment to support the CKD patient over the world [1–3]. Furthermore, the main component in the equipment of hemodialysis is the membrane which can reject toxic compounds (creatinine and urea) and save the essential compound (protein and vitamins) in the blood selectively [4]. Besides, the membrane should be biocompatible, selective, and non-toxic [5].

Polysulfone (PSf) is material that normally is used as a hemodialysis membrane. Because PSf has good mechanical strength, good thermal stability, and inert in the chemical compounds but PSf is hydrophobics and less functional group[6–8] Finally, many researchers feel that PSf was needed to modify with the other compounds to be more hydrophilic and more functional group [8–12].

In addition, there are so many factors that affect a transport process for example pore size, molecule size, drag force, and surface area. While, if it looked to the molecular perspective, the functional group plays a significant role to improve the ability of the membranes. More details, the interaction between the membrane and the transport molecule need to study deeply. Currently, the use of computational chemistry is needed to give details explanations of the interactions at the molecular



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level accurately. Costa et al. (2018), has investigated the interaction between dimer chitosan and alginate to know polyelectrolyte complex [13]. In transport phenomena in the membrane, the use of a theoretical approach gives more details about energetic, geometric, and electronic parameters in a molecular structure model for the interaction of target molecules with the membrane by obtaining [9–10]. because of the highest cost to simulate polymer molecules, polymer normally is calculated in the dimer structure [7, 11–14].

This paper focuses on the studies of molecular interaction between PSf with creatinine and urea for the application of hemodialysis membrane at the molecular level. The objective of this theoretical study is to identify the possible interactions start from geometry optimization to determine the energetic and electrical parameter of interaction. The Density Functional Theory (DFT) was employed. This study can lead to prove why the PSf membrane needs to modify.

## 2. Computational details

Density Functional Theory was used for calculation in this research. The calculation begins by optimizing the polysulfone, urea, and creatinine structure to find their minimum energy, individually. Furthermore, the interaction of PSf-Creatinine and PSf-Urea was calculated to reach the most stable interaction and get the minimum energy. After the optimization, The task of frequencies was applied to clarify that the molecule or complexes were stable molecules. A positive value of frequencies means that a molecule has already stable [7, 12–14, 19]. The equation below was the equation to calculate interaction energy:

$$E_{\text{int}} = E_{\text{PSf/urea}} - (E_{\text{PSf}} + E_{\text{urea}}) + E_{\text{BSSE PSf/urea}} \quad (1)$$

$$E_{\text{int}} = E_{\text{PSf/creatinine}} - (E_{\text{PSf}} + E_{\text{creatinine}}) + E_{\text{BSSE PSf/creatinine}} \quad (2)$$

Where  $E_{\text{PSf/urea}}$  and  $E_{\text{PSf/creatinine}}$  are the stable energies of chitosan-urea and chitosan-creatinine complexes, respectively. The interaction which occurs in the PSf and urea or creatinine is non-covalent interaction which is hydrogen bonding [22]. The calculation of the interaction energy help to find the kind of hydrogen bond interaction whether weak, medium, or strong. All of the investigations were calculated by Chemcraft [23], Gauss View graphical interface, NWChem [24], and GAMESS [25]. All calculation was performed by 6-31g\*\* basis set and DFT method with the hybrid quality of Becke three-parameter exchanges Lee et al. of correlation functional (B3LYP) method.

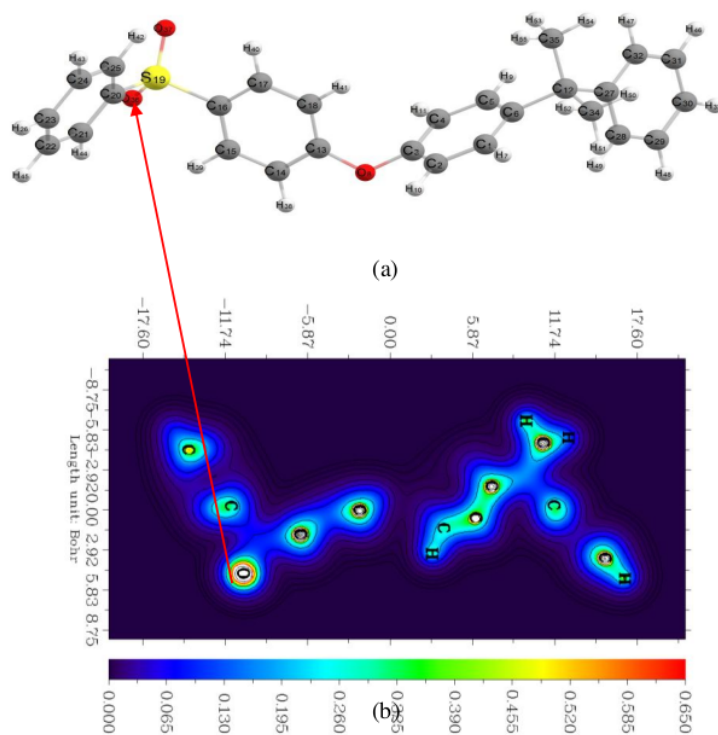
## 3. Results and discussion

### 3.1. Structure of PSf, urea, creatinine

The optimization of a molecule was the first step before investigated the other parameters. Furthermore, it is used to obtain an optimized geometry that has been built manually. Hence, the GAMESS program was applied to calculate the structure of PSf, urea, and, creatinine individually. The figure of optimizing molecule PSf, Creatinine, Urea, can be seen in Figure 1, Figure 2, Figure 3, respectively.

Polysulfone (PSf) was the synthetics polymer that generally was applied in the hemodialysis membrane [26][6]. The figure shows that the structure of Polysulfone was not linear. It was probably because three different types were linking for the ring of benzene which was O (O9), SO<sub>2</sub> (S19), and C3H7 (C12). Moreover, the Ether group in PSf will give a free rotation in this molecule which enhances the mechanical strength of polymer and also significantly decrease of melting point. Otherwise, the Sulfonyl group can attribute the stability of the polymer. In this case, the electron from the aromatic ring will be attracted by the sulfone group, so it causes electron deficiency. This statement was supported by figure 1.b which shows the electronics parameters of PSF-structure. The red side to the blue side indicated the most to the lowest of total density electrons which means that red is negative side and blue is the positive side. The figure 1b also shows the site active which was possible to make interaction with urea and creatinine. O36 is the most negative one, whereas O8 and

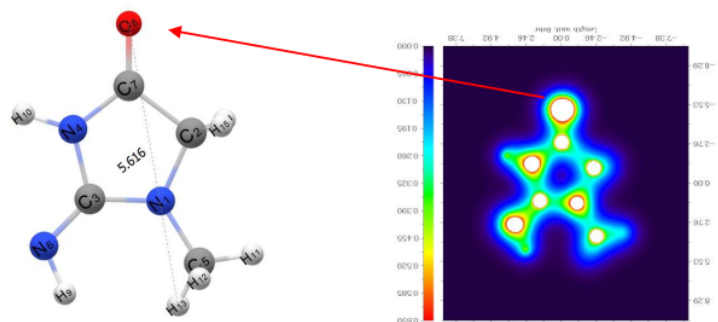
C13 are positive and more electrophilic. Hence, O8 and C13 are the possible sites to make interactions with urea and creatinine which have many negative sites.



**Figure. 1** (a) Optimize geometry of PSf (b) MEP of PSf

### 3.2. Structure of creatinine

Creatinine was a toxic compound result of muscle metabolism which have to reject from the blood by kidneys. Creatinine level in humans is generally 0.7-1.2 mg/dL. An exceed of creatinine concentration enervates the activity of kidneys [27]. However, there is a hemodialysis membrane which helps the people who suffer a CKD, the researcher must know the size and properties of creatinine



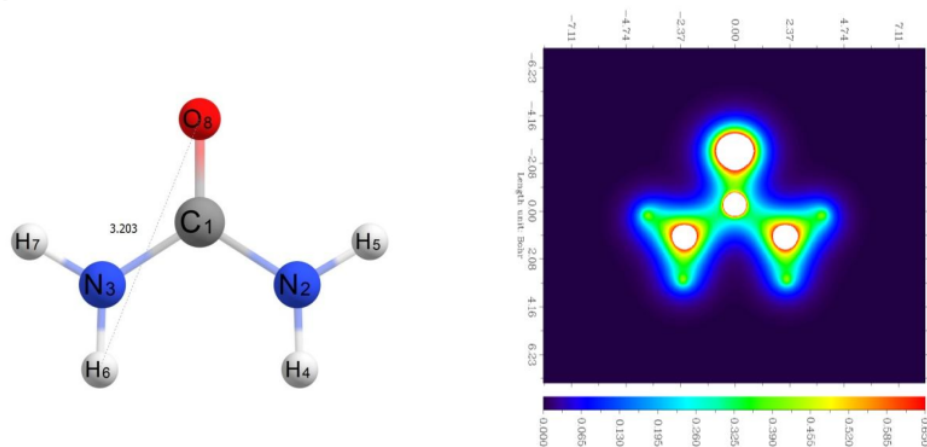
**Figure. 2** (a) Optimize Geometry of Creatinine (b) MEP of Creatinine

In this study, we have obtained the size of the creatinine and studied its properties (see Figure 2). Figure 2. It illustrates that the size of creatinine is about 5.616 Å. The size was obtained by measuring the longest distance in H13 to O8. According to the data, it can be inferred that the pore size of the hemodialysis membrane has to be bigger than 5.616 Å. Besides, this study also evaluated the electronic structure of creatinine. However, the electronics parameter also evaluated for creatinine to determine the active site which possibly can make interaction with the other molecule particularly PSf. The figures describe that creatinine has several active sites which are the potential to make interaction. The interaction can occur in the N6-H9, N4 –H10, and methyl in C5 if the opponents have a negative charge, while, if the opponent's molecule has a more positive charge, the interaction will be through O8. So, it can be inferred that the interaction will happen in many sites depend on the other molecule, although in the case of creatinine-psf interaction, it will happen in through N6-H9 and N4 –H10.

### 3.3. Structure of urea

Urea is the other molecule that must be rejected from the body by hemodialysis membrane. Because Urea is a dangerous compound if there are more than 40 mg/dL in the body. Furthermore, urea will rise if there is no rejection because urea is the final product of protein metabolism in the human body [28]. Not only bigger than creatinine, but the pore size of the membrane also must be bigger than urea.

According to Figure 3a, the urea has a size approach of 3.203 Å which is smaller than creatinine. This data has suggested that the hemodialysis membrane should have a diameter of pore bigger than 5.358 Å. In the previous study, some people have made the PSf membrane with pore size bigger than 5.358 Å [2, 29–31]. According to creatinine and urea size, it can be predicted that urea faster to transport in the PSf membrane. This result was linear with Lusiana et al (2013) that urea was easier to reject in PSf derivative membrane than creatinine [5]. In addition, Figure 3b illustrates that the possible interaction is in the amine group ( $-NH_2$ ). Finally, to know a more accurate conclusion, the probing of interaction between PSf and creatinine or urea will be further discussed.



**Figure. 3** (a) Optimize geometry of urea (b) MEP of urea

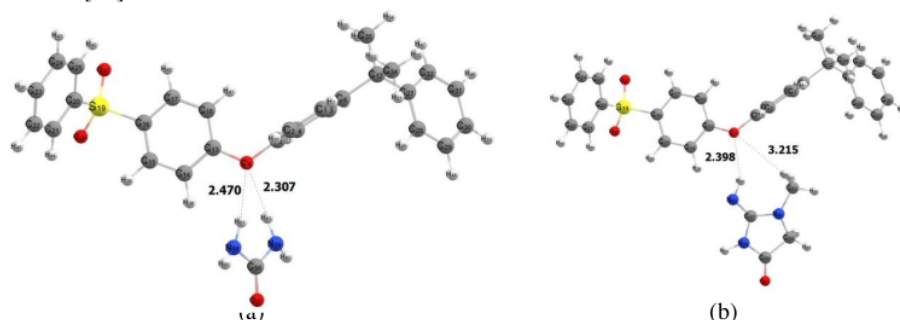
### 3.4. Interaction energy

Intermolecular interaction is a well-known study in understanding phenomena atom and molecule as a system of chemistry [32–37]. In these cases, interaction energy was determined to know how strong the interaction between membrane and molecule target. A higher value of interaction energy ( $E_{int}$ ) shows the stronger binding among two or more molecules. Furthermore, this study focus on the interactions that occur in transport phenomena by using a membrane. The other study before, proton



and electron transfer on the Proton Exchange Membrane Fuels Cells was evaluated to describe the interaction which occurs in that membrane [38].

The calculation was investigated at the B3LYP/6-31G\*\* level and corrected by zero-point energy (ZPE) and basis set superposition error (BSSE). However, there were two hydrogen bonds that form between PSf and urea by (O8...H63-N59 = 2.2307 Å) and (O8...H61-N58 = 2.470 Å). Whereas, The interaction energy of PSf and urea are about - 6.31021 kcal/mol. This data includes the weak hydrogen bonds [38].



**Figure. 4** Interaction of ; (a) PSf - urea (b) PSf - creatinine

The interaction energy value of the PSf-creatinine complex was -3.87571 kcal/mol which exists in O8...H65-N63 (2.398 Å). It is classified in the weak hydrogen bond similar to PSf-Urea interaction. However, the strong hydrogen bond causes the acceleration of transport in the membrane compare but the strong hydrogen bond can also make fouling in the membrane. On the other hand, the weaker hydrogen bond with urea and creatinine cannot improve the ability of the membrane [41–46]. Thus, the medium hydrogen bond is the best way to enhance the ability membrane. Moreover, These results give an explanation that PSf-urea interaction is stronger than PSf-creatinine. So, base on the size and the interaction data, urea is easier to transport than creatinine in the PSf membrane. In conclusion, PSf is a potential material for the membrane, although it is substantial to modify the PSf with the other materials to give a more functional group and to make stronger interaction with the molecular target.

### 3.5. NBO analysis

NBO analysis is the method that uses the second perturbation theory to determine the stabilization energy ( $E^2$ ) [45]. Furthermore, this analysis can also use to investigate the type of hydrogen bond which is essential for study the interaction, particularly in the transport phenomena [46]. Hence, NBO analysis supports the energy interaction to judge the force of hydrogen bonding interaction. In this study, The NBO analyses are applied to investigate the H-bonds within the complex of PSf-Urea and The complex of PSf-creatinine.

**Table 1.** NBO analysis of PSf-urea interaction

No	9 Donor (L) NBO	Accepter (NL) NBO	$E^2$ kcal/mol	$E(NL)-E(L)$ a.u.	$F(L,NL)$ a.u.
From PSf to Urea					
1	1 LP (1) O 8	BD*(1) N 58- H 61	1.26	0.99	0.032
2	LP (1) O 8	BD*(1) N 59- H 63	1.71	1	0.037
3	LP (2) O 8	BD*(1) N 58- H 61	0.21	0.83	0.012

4	<sup>1</sup> LP (2) O 8	BD*(1) N 59- H 63	1.19	0.84	0.028
From Urea to PSf					
5	LP (1) N 58	<sup>1</sup> BD*(1) C 14- H 38	1.59	0.76	0.031
6	BD (1) N 58- H 61	BD*(1) C 14- H 38	0.08	1.09	0.008
7	BD (1) N 58- H 61	RY (1) H 38	0.22	1.33	0.015

In contrast, it can be seen from Figure 4a, and table 1. that the hydrogen bond between PSf and urea present in O8...H63-N59 and O8...H61-N58. Then, table 1 depicts the stabilization energy from donor to acceptor which occurs from PSf to urea or from urea to PSf. Furthermore, Atom O8 in urea has two kinds of LP as a donor, while urea has BD\*(1)N 59 - H63 and BD\*(1) N58 -H61 as acceptor. Based on table 1. It is clear that the stabilization of LP (1) O8 to BD\*(1) N 59- H 63 is the highest value by 1.74 kcal/mol. moreover, the averages of stabilization energy between PSf and Urea are no more than 2 kcal/mol. hence, it can be concluded that the interaction between PSf and urea is the very week hydrogen bond interaction [46].

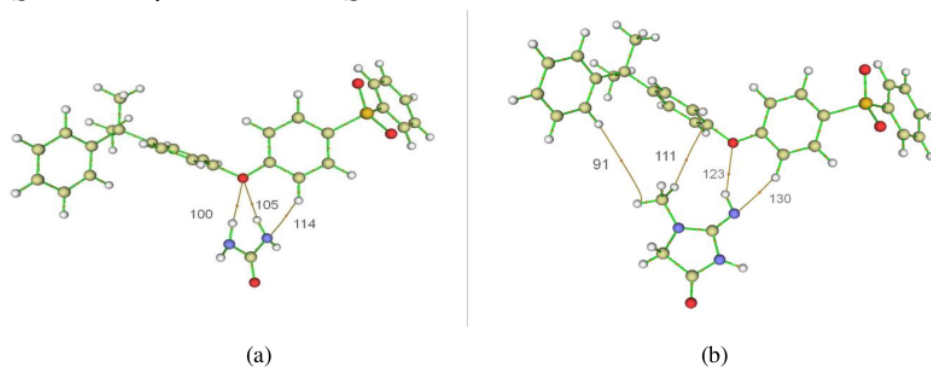
On the other hand, the interaction between PSf and Creatinine is also categorized as a very week hydrogen bond because the number of stabilization energy among PSf and creatinine is no more than 4 kcal/mol. According to the maharani (2016), the interaction which is classified in the very week hydrogen interaction is the interaction that has stabilization energy no more than 4 kcal/mol [47]. furthermore, the interaction between PSf and creatinine appears in the LP (O8)... BD\*( 1) N 63- H 65 which has the stabilization energy by 1.85 kcal/mol. the highest energy stabilization occurred in the LP (1) N 63 to BD\*(1) C 14- H 38 is by about 2.21 kcal/mol. however the highest stabilization energy in the interaction among PSf-creatinine higher than PSf-Urea, but the average of stabilization energy between PSf-Urea higher than PSf-creatinine. So, Based on the NBO analysis data, it can conclude that urea easier moves through the PSf membrane than creatinine. This data supports the interaction energy data in the previous analysis.

**Table 2.** NBO analysis of PSf-creatinine interaction

No	<sup>9</sup> Donor (L) NBO	Acceptor (NL) NBO	<sup>18</sup> E <sup>2</sup> kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
From PSf to Creatinine					
1	<sup>1</sup> LP (1) O 8	<sup>1</sup> BD*(1) N 63- H 65	1.85	0.99	0.038
2	LP (2) <sup>5</sup> 8	<sup>18</sup> BD*(1) N 63- H 65	0.22	0.83	0.012
3	BD (2) C 2- C 3	BD*(1) C 62- H 68	0.21	0.71	0.011
4	BD (1) C 14- H 38	BD*(1) C 57- N 63	0.05	1.12	0.007
5	BD (1) C 14- H 38	BD*(2) C 57- N 63	0.18	0.51	0.008
6	BD (1) C 14- H 38	RY (2) N 63	0.11	1.39	0.011
From Creatinine <sup>17</sup> PSf					
7	LP (1) N 63	BD*(1) C 14- H 38	2.21	0.81	0.038
8	<sup>5</sup> BD (1) C 57- N 63	RY (1) H 38 <sup>17</sup>	0.1	1.55	0.011
9	BD (2) C 57- N 63	BD*(1) C 14- H 38	0.56	0.82	0.019
10	BD (2) C 57- N 63	RY (1) H 38	0.12	1.11	0.01
11	<sup>1</sup> BD (1) N 63- H 65	BD*(1) C 14- H 38	0.17	1.05	0.012
12	BD (1) N 63- H 65	RY (2) C 14	0.06	1.34	0.008
13	BD (1) N 63- H 65	RY (1) H 38	0.31	1.34	0.018



### 3.6. Quantum theory atom in molecule QTAIM



**Figure. 5** Bond critical point (a) PSf-Urea (b) PSf-creatinine

In 1990, a saddle point of electron density between two atoms that form a chemical bond has been illustrated by Brader as bond critical point (BCP) [48]. Furthermore, quantum theory atom in molecule (QTAIM) analysis can generate the important parameters such as Laplacian ( $\nabla^2 \rho$ ), ellipticity  $\epsilon_{(BCP)}$ , Electronic energy density ( $H$ ), kinetic energy density ( $G_{(BCP)}$ ), potential energy density ( $V_{(BCP)}$ ) [49]. The equation of the parameters at the BCP is given by the following equation:

$$\nabla^2 \rho = \lambda_1 + \lambda_2 + \lambda_3,$$

$$H_{(BCP)} = G_{(BCP)} + V_{(BCP)}$$

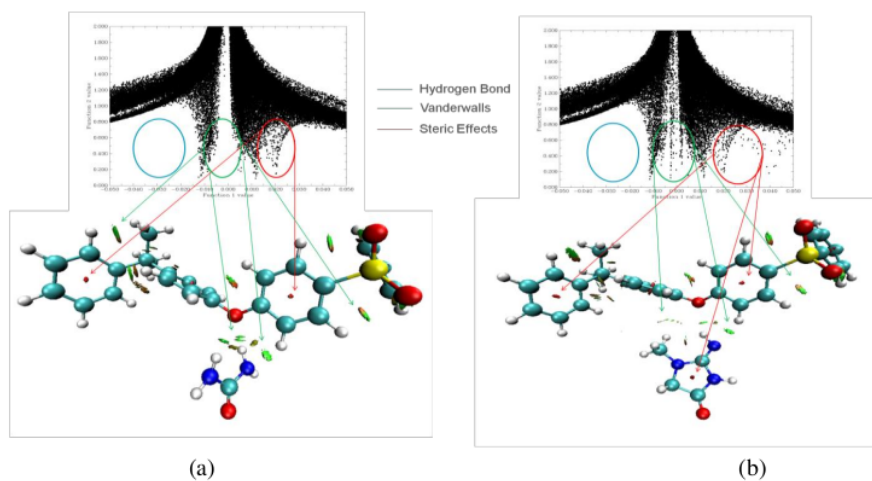
Brader's theory state that  $\nabla^2 \rho$  and  $H_{(BCP)}$  can be used to determine the type of interaction where  $\nabla^2 \rho$  (+) and  $H_{(BCP)}$  (+) illustrate The weak covalent interactions [12, 49]. Furthermore, the ratio of  $|V/G|$  can be also generated to classify the type of interactions. Weak interactions are depicted with  $|V/G| < 1$ , medium interactions  $1 < |V/G| < 2$ , and strong interactions  $|V/G| > 2$  [50][51]. The QTAIM parameter was presented in table 3.

**Table 3.** QTAIM parameters of PSf-creatinine and PSf-urea interaction

BCP	$\nabla^2 r$	$G_{(BCP)}$	$H_{(BCP)}$	$-V_{(BCP)}$	$ V/G $	EHB (kcal/mol)
PSf-Creatinine						
91	7.11E-04	1.22E-04	5.63E-05	6.53E-05	5.37E-01	-0.02047929
111	8.30E-03	1.57E-03	5.04E-04	1.07E-03	6.79E-01	-0.33484901
123	3.44E-02	8.13E-03	4.67E-04	7.66E-03	9.43E-01	-2.40420841
130	3.25E-02	7.56E-03	5.70E-04	6.99E-03	9.25E-01	-2.19335118
PSf-Urea						
100	3.87E-02	9.60E-03	7.67E-05	9.52E-03	9.92E-01	-2.98671594
105	3.25E-02	7.35E-03	7.65E-04	6.58E-03	8.96E-01	-2.06574602
114	2.30E-02	5.19E-03	5.53E-04	4.64E-03	8.94E-01	-1.45624659

According to figure 4e and Table 3., there are three BCP which present in the interaction between PSf Urea. This BCP was labeled with 100, 105, and 114. Overall, it can be seen that all BCP have a positive  $H_{(BCP)}$  and positive  $\nabla^2 r$  which indicates the weak covalent interaction. Furthermore, the ratio of  $|V/G|$  is no more than 1 which also indicates that the interaction between PSf and Urea is weak interaction. Likewise,  $E_{HB}$  is the hydrogen bond energy which is half of  $V_{(BCP)}$  [50]. The strongest interaction occurs in the BCP number 100 which has the highest hydrogen bond by about -2.98 kcal/mol. whereas, the other interaction occurs in the BCP 105 and 114 which have the hydrogen bond energy by about -2.06 kcal/mol and -1.46 kcal/mol respectively.

There are 4 BCP in the interaction between PSf and creatinine. As same as PSf-urea interaction, The data shows that the interaction of PSf and creatinine is also the weak interaction. All of  $\nabla^2 r$  and  $H_{(BCP)}$  value are positive which indicate the weak interaction. This data also supported by the ratio of  $|V/G|$  which the value is under one. There are 2 BCP which have a hydrogen bond energy more than 2. This is BCP numbers 123 and 130 by about -2.40 kcal/mol and -2.19 kcal/mol respectively. The BCP number 123 and 130 have a value which is different to number 91 and 111 significantly because the interaction in number 123 and 130 are the interaction between atom hydrogen and the atom having the high electronegativity such as N and O, whereas number 91 and 111 are the hydrogen-hydrogen interaction and hydrogen carbon interaction respectively [52–54]. Furthermore, although PSf-creatinine interaction has 4 BCP while the interaction of PSf-urea has 3 BCP, the average or hydrogen bond energy in the PSf-urea is higher than the interaction PSf-creatinine. Hence, These analysis has supported the interaction and size data where urea is easier to transport through the PSf membrane than creatinine.



**Figure 6.** The RDG/sign( $\lambda^2$ ) $\rho$  for (a) PSf-Urea (b) PSf-Creatinine

On the other hand, The scatter of reduced density gradient tRDG vs sign( $\lambda^2$ ) $\rho$  can be used to analyze the type of interaction, in particular, the noncovalent interaction such as hydrogen bond and Vanderwall interaction [48,55]. the Scatter of RDG was generated by multywn software and visualized by VMD. In addition, Johnshon et al (2010) define the RDG equation which presented in the following equation [56].

$$RDG(r) = \frac{1}{2(3\pi^2)^{1/3}} \frac{|V\rho(r)|}{\rho(r)^{4/3}}$$

Figure 6. display the scatter graph and isosurface of complex PSf-Urea and creatinine where RDG define as function 2 or ordinate and  $\text{sign}(\lambda_2)\rho$  define as function 1 or absis. Furthermore, it can be seen that there is no hydrogen bond interaction in both PSF-creatinine complex or PSf urea. hence, this indicates that the interaction between PSf with urea and creatinine is a very weak interaction. otherwise, Vanderwall interaction dominated in this interaction which is presented in the green circle. Moreover, it can be seen that there is a steric effect in the creatinine which caused the interaction with PSf to be weak. While there is no steric effect in the urea so the interaction will stronger. This data was supported by previous analysis where urea has a stronger interaction with PSf than creatinine. In conclusion, both urea and creatinine just interact weakly with PSf, however, urea can make stronger interaction with PSf than urea. hence, PSf still needs to modify with the additive which can enrich the functional group so it can make strong interaction with urea and creatinine and enhance the transport performance.

#### 4. Conclusion

The interaction between PSf with creatinine and urea are -3.87 kcal/mol and -6.31 kcal/mol, respectively. While, the size of urea is smaller than creatinine by 3.2 Å and 5.6 Å, respectively. Furthermore, NBO analysis and QTAIM analysis shows that both of the interaction PSf-creatinine and PSf-urea are very weak interaction. It can be concluded that urea is easier to transport in the PSf membrane than creatinine during the hemodialysis process. Whereas PSF still need to modify with the additive to enrich the functional group, hence it can make stronger interaction and enhance the transport performance in the hemodialysis system

#### Acknowledgments

Gratefully acknowledge to Indonesian General Directorate<sup>[20]</sup> Higher Education, which has funded this research and technology on the funding scheme 2018 and 2019.

#### Conflict of Interest

The authors declare no conflict of interest.

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