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THEORETICAL STUDY OF THE GLYCEROL ADSORPTION FROM THE BIOFUEL OVER TiO_2 CATALYTIC SURFACE

Abstract. The traditional fuel such as petroleum, natural gas and others could be partially replaced by biodiesel. At the same time, the main problem for the mass production of biofuel is linked to the glycerol which is a by-product of biodiesel and leads to many chemical and engineering challenges. In this regard, there are various methods to extract glycerol from biofuel including implementation of solvents, catalysts, and others. Herein, we performed quantum-chemical computational study on the titanium (IV) oxide-based catalyst activity for the adsorption of glycerol from biofuel in the first part of our work. Then, we performed quantum-chemical computational investigation on the transformation of glycerol into valuable product acrolein. The result revealed the presence of strong chemical interaction between titanium (IV) oxide and glycerol of biofuel in the adsorption process.

Key words: titanium (IV) oxide, glycerol, biofuel, adsorption, quantum chemistry.

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TiO_2 КАТАЛИТИКАЛЫҚ БЕТІ АРҚЫЛЫ БИООТЫННАН ГЛИЦЕРОЛДЫ АДСОРБЦИЯЛАУ ПРОЦЕССІН ТЕОРИЯЛЫҚ ТҰРҒЫДА ЗЕРТТЕУ

Аннотация. Дәстүрлі отын, мысалы, мұнай, табиғи газ және т.б. ішінара биодизельмен ауыстырылуы мүмкін. Сонымен қатар, биоотынның жаппай өндірісінің негізгі проблемасы биодизельдің жанама өнімі болып табылатын және көптеген химиялық және инженерлік қиындықтарға әкелетін глицеринмен байланысты. Осыған байланысты биоотыннан глицерин алудың әртүрлі әдістері бар, соның ішінде еріткіштерді, катализаторларды және т.б. Жұмыстың бірінші бөлігінде биоотыннан глицеринді адсорбциялау үшін титан (IV) оксидіне негізделген катализатор белсенділігіне кванттық химиялық есептеу жүргізілді. Одан кейін глицериннің акролеиннің құнды өніміне айналуы бойынша кванттық химиялық есептеу жүргізілді. Нәтиже адсорбция процесінде биоотынның титан (IV) оксиді мен глицерин арасында күшті химиялық әсерлесудің болуын көрсетті.

Түйін сөздер: титан (IV) оксиді, глицерин, биоотын, адсорбция, кванттық химия.

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ТЕОРЕТИЧЕСКОЕ ИССЛЕДОВАНИЕ АДСОРБЦИИ ГЛИЦЕРИНА ИЗ БИОТОПЛИВА ЧЕРЕЗ КАТАЛИТИЧЕСКУЮ ПОВЕРХНОСТЬ TiO_2

Аннотация. Традиционное топливо, такое как нефть, природный газ и другие может быть частично заменено биодизелем. В то же время основная проблема массового производства биотоплива связана с глицерином, который является побочным продуктом биодизеля и приводит к многочисленным химическим и инженерным проблемам. В связи с этим существуют различные способы извлечения глицерина из биотоплива, в том числе с применением растворителей, катализаторов и др. Здесь мы провели квантово-химическое вычислительное исследование активности катализатора на основе оксида титана (IV) для адсорбции глицерина из биотоплива в первой части нашей работы. Затем мы провели квантово-химическое вычислительное исследование превращения глицерина в ценный продукт акролеин. Результат предполагал наличие сильного химического взаимодействия между оксидом титана (IV) и глицерином биотоплива в процессе адсорбции.

Ключевые слова: оксид титана (IV), глицерин, биотопливо, адсорбция, квантовая химия.

Introduction. The generation of biodiesel is rising in the global market in order to replace a traditional energy source including petroleum, natural gas and others. At this level, there are many existing advantages of biofuel including decreasing in greenhouse gas emission, cheaper in contrast with petroleum and natural gas, less-flammable, renewable and others (Liang et al., 2013:139-145; Ferrero et al., 2016:495-503; Baroutian et al., 2013:911-916; Cheng et al., 2011:3541-3549). However, the accumulated generation of glycerol as a by-product during the biofuel production is a main challenge. The glycerol is an unwanted impurity in the biofuel content that leads to i) difficulty during the storage, ii) fouling of the injector, iii) durability problem of engine and others (Chhabra et al., 2021:3381-3392; Taufiqurrahmi et al., 2011:10686-10694; Long et al., 2022:109-119; Santana et al., 2021:9185). Herein, there are much ongoing research related to the transformation of glycerol into high value product. In this regard, there are exist various methods to convert a glycerol into high value product such as i) esterification process, ii) hydrogenolysis method, iii) polymerization, iv) etherification method, and finally v) dehydration method (Bora et al., 2016:560-568; Li et al., 2016:98-194; Yuvaraj et al., 2019:301-307).

Due to this, the dehydration of glycerol into acrolein is an important method for nowadays. This process can be achieved by the presence of solid catalysts. The final product which is named as an acrolein is a crucially important chemical materials that could be implemented in the acrylic acid production (Bateni et al., 2017:668-690). Herein, acrylic acid is an important compound to get various polymers and an important starting material for the methionine synthesis. Moreover, the conversion of glycerol to acrolein is achieved by the removal of two water molecules over titanium (IV) oxide catalyst and others (Crossley et al., 2010:68-72; Liu et al., 2018:375-380).

The glycerol has adjacent three hydroxyl functional groups, and consequently, it is the simplest chemical structure to study glucose and other types of sugars in the computational world. Consequently, a lot of experimental works were performed to study the transformation of glycerol to acrolein. For instance, the generation of acrolein from glycerol by titanium oxide catalyst is studied in more details (Gueddida et al., 2020:20262-20269; Chakrabortty et al., 2020:675-690; Gao et al., 2009:356-361; Lee et al., 2013:6-11; Alonso et al., 2010:1493-1513). Titanium (IV) oxide has a three crystalline phase such as i) rutile, ii) anatase, and iii) brookite. Herein, titanium (IV) oxide with anatase structure is an important compound in the field of catalysts. Moreover, the anatase structured titanium (IV) oxide is having different types of advantages such as thermally stable, less expensive, safe, and can be reused (Jabraoui et al., 2019:882-892; De lima et al., 2020:4124-4130; Huang et al., 2016:490-497).

In this work, we are going to investigate titanium (IV) oxide’s absorption property of glycerol from biodiesel. Moreover, the conversion process of glycerol into high value acrolein product by titanium (IV) oxide catalyst will be investigated computationally as well. We will use HyperChem computational package and PM3 approach to explore molecular details of adsorption and transformation processes. In general, the electronic structures, electrostatic maps, orbitals, bond length, and interaction energies related to the adsorption of glycerol from biodiesel by titanium (IV) oxide and transformation of glycerol to acrolein will be explored in this work.

Research material and methods. HyperChem with PM3 method was implemented for quantum-chemical calculations. It is possible to evaluate the interaction between the titanium atom in TiO2 and the oxygen atoms in the glycerol molecule while the glycerol was selected as an unwanted impurity of biodiesel, while the methyl linoleate was a model for biodiesel. Moreover, acrolein was selected as a computation model for high value product which was obtained during the transformation of glycerol. The calculated parameters are electronic structures, electrostatic maps, orbitals, bond length, and interaction energies. The 2D structures of above-mentioned compounds for titanium oxide, glycerol, acrolein, and methyl linoleate are illustrated in Figure 1.

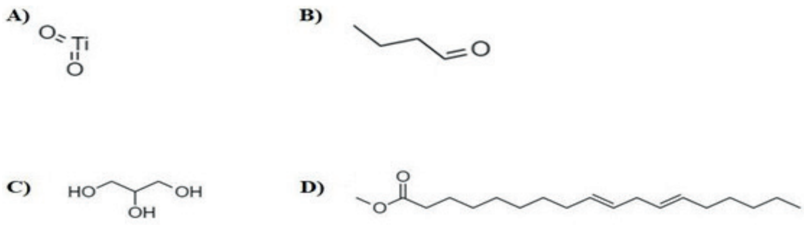

Figure 1. The 2D chemical structures of A) titanium (IV) oxide, B) acrolein, C) glycerol, and D) methyl linoleate.

Meanwhile, the adsorption and production energies were calculated using below given formula:

$$E_{adsorption} = E_{(TiO2)+Glycerol+Biofuel)} - (E_{(Glycerol)} + E_{(Biofuel)} + E_{(TiO2)})$$

$$E_{Production} = E_{(TiO2+Acrolein+Methyl\ linoleate)} - (E_{(Acrolein)} + E_{(Biofuel)} + E_{(TiO2)})$$

The models for computation were shown in Table 1.

Table 1 – The designed simulation system for study of glycerol adsorption from biofuel by titanium (IV) oxide and a transformation of glycerol into acrolein

Titanium (IV) oxide	Glycerol	Methyl linoleate	Acrolein
1	-	-	-
-	1	-	-
-	-	1	-
-	-	-	1
1	1	1	-
1	-	1	1

As found from table 1, the pure titanium oxide, glycerol, methyl linoleate, and an acrolein as a catalyst, impurity, biofuel, and high value produces were simulated firstly. Next, a mixture of titanium (IV) oxide with glycerol, and methyl linoleate was simulated as an impure biofuel purification process by titanium (IV) oxide catalyst. After that, the mixture of titanium oxide catalyst with glycerol, methyl linoleate, and an acrolein was simulated as a model for the acrolein synthesis process.

Results. The intermolecular interaction of absorption process of glycerol by titanium (IV) oxide from biofuel. Firstly, we studied the adsorption of glycerol from biofuel using a titanium (IV) oxide-based catalyst surface. The results were illustrated from Figure 2 to Figure 4, and in Table 2.

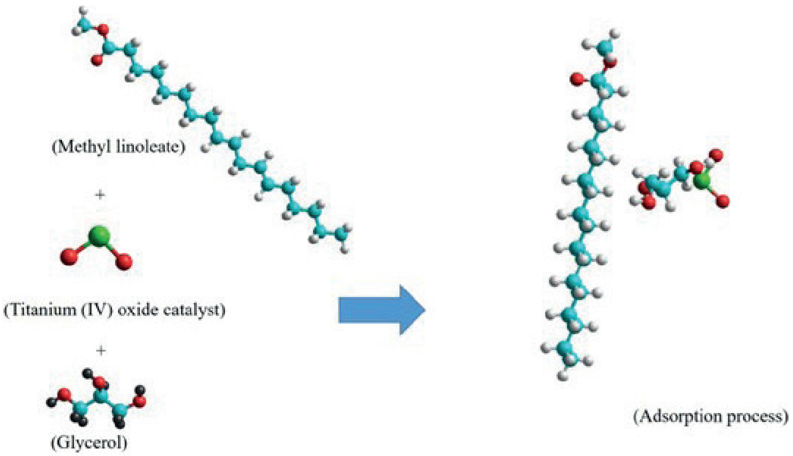

Figure 2. The electronic structures of titanium (IV) oxide, glycerol, and methyl linoleate.

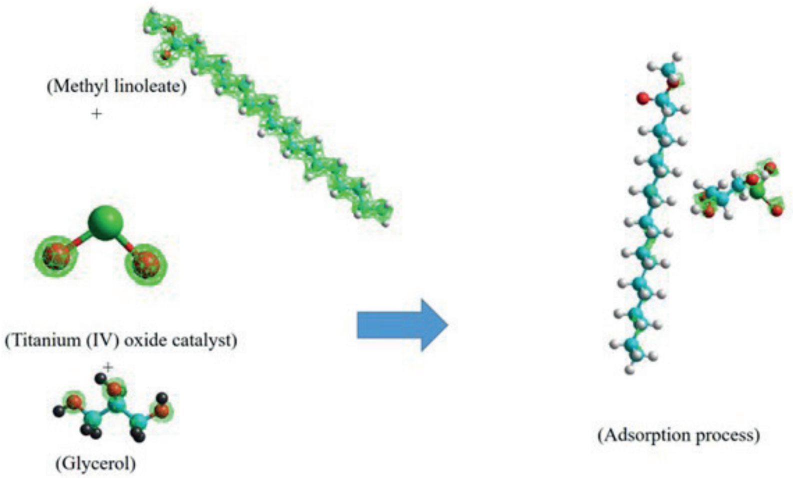

Figure 3. The molecular electrostatic maps of titanium (IV) oxide, glycerol, and methyl linoleate.

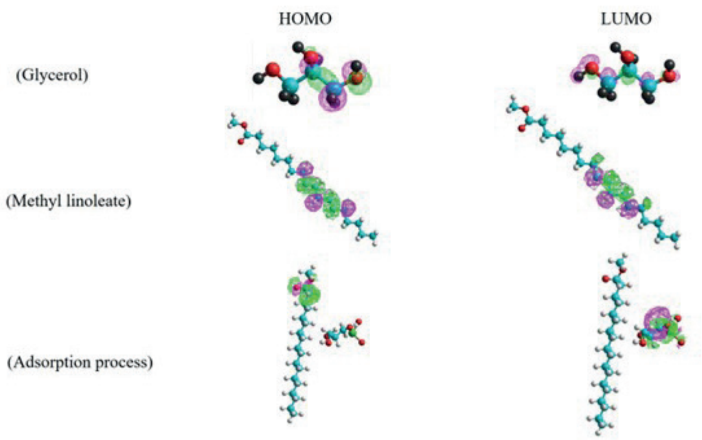

Figure 4. The molecular orbitals of titanium (IV) oxide, glycerol, and methyl linoleate.

Table 2 – Energies for titanium (VI) oxide, glycerol, and methyl linoleate. Unit: kcal/mol

	Glycerol	Biofuel	Titanium (IV) oxide + Glycerol + Biofuel
Energy (kcal/mol)	-31376.50	-77595.70	-126605.00

The intermolecular interaction of transformation process of glycerol into acrolein by titanium (IV) oxide from biofuel. Secondly, we studied the intermolecular interaction of acrolein a produced high value product on the titanium (IV) oxide catalytic surface in the presence of pure biofuel. The results were illustrated from Figure 5 to Figure 7, and in Table 3.

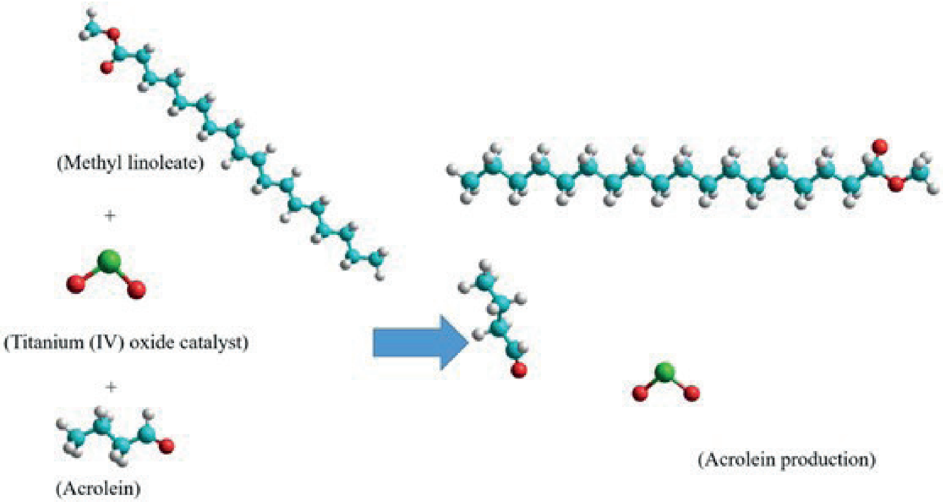

Figure 5. The electronic structures of titanium (IV) oxide, acrolein, and methyl linoleate.

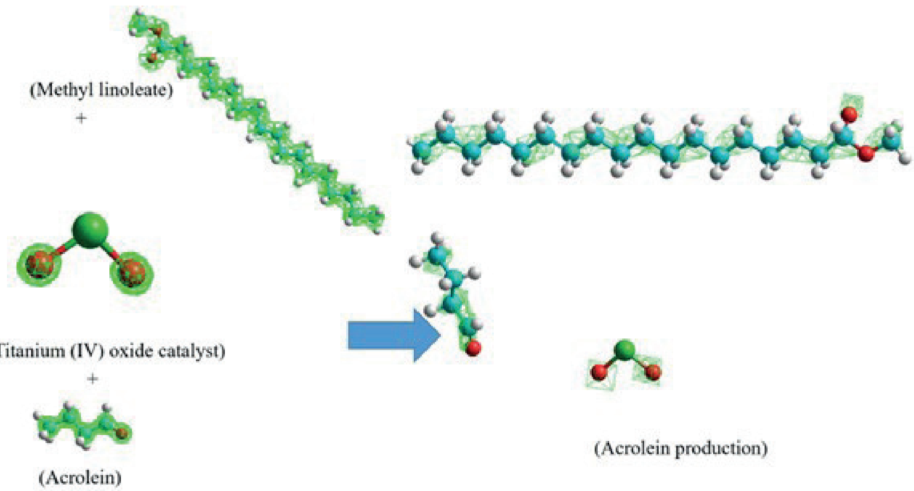

Figure 6. The molecular electrostatic maps of titanium (IV) oxide, acrolein, and methyl linoleate.

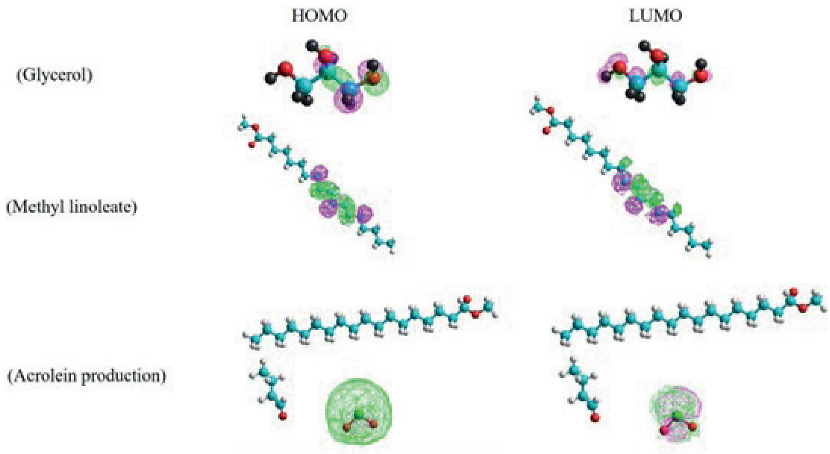

Figure 7. The molecular orbitals of titanium (IV) oxide, acrolein, and methyl linoleate.

Table 3 – Energies for titanium (VI) oxide, acrolein, and biofuel model (methyl linoleate). Unit: kcal/mol

	Acrolein	Biofuel	Titanium (IV) oxide + Acrolein + Methyl linoleate
Energy (kcal/mol)	-20502.60	-77595.70	-115576

Discussion. In the first part of our work, we studied the optimized structures for adsorption process in detail as can be seen in Figure 3. From Figure 3, we can note that a titanium metal is chemically interacting with an oxygen atom of glycerol in the presence of methyl linoleate as a model biofuel. Herein, we can note that the connection between oxygen atom of glycerol and titanium metal is a main driving force for the adsorption process.

Next, we studied the distribution of molecular electrostatic maps over a titanium oxide surface as can be seen in Figure 4. From Figure 4, we can note that the charges are located around oxygen atoms of glycerol and a titanium (IV) oxide.

From Figure 5, the HOMO-LUMO orbital distribution for adsorption process of glycerol from biofuel by titanium (IV) oxide is illustrated. From there, we can note that the HOMO orbitals are distributed around biofuel part, while the LUMO energies are localized around titanium (IV) oxide and glycerol compounds.

Next, we calculated the adsorption energy as below:

$E_{adsorption}$ = -126605.00 – (- 31376.50 – 77595.70 - 15646) = -1986.80 kcal/mol, which means a higher adsorption by titanium (IV) oxide.

In the second part of our work, we studied the optimized structures for conversion process in detail as can be seen in Figure 5. From Figure 5, we can note that a titanium metal is less chemically interacting with an acrolein in the presence of methyl linoleate as a model biofuel. Herein, we can note that the result of conversion process is a generation of acrolein.

Next, we studied the distribution of molecular electrostatic maps over a titanium oxide surface as can be seen in Figure 6. From Figure 6, we can note that the charges are located around entire biofuel, acrolein, and titanium (IV) oxide catalyst.

From Figure 7, the HOMO-LUMO orbital distribution for adsorption process of glycerol from biofuel by titanium (IV) oxide is illustrated. From there, we can note that both HOMO and LUMO orbitals are located around titanium (IV) oxide.

Next, we calculated the product generation energy as below:

$E_{production}$ = -115576.00 – (- 20502.60 – 77595.70 - 15646) = -1831.70 kcal/mol, which means a generation of acrolein as a product.

Conclusion. In this study, the adsorption of glycerol from biodiesel by a titanium (IV) oxide catalyst was investigated in the first part of our work, while the transformation of glycerol into acrolein was studied in the second part of our work.

The result of our first computational study yielded that there were strong chemical bond present between titanium cation of titanium (IV) oxide and an oxygen anion of glycerol compound of biodiesel. This illustrated a strong absorption ability of glycerol on titanium (IV) oxide catalyst surface in the presence of methyl linoleate as a biofuel model.

The result of our second computational work yielded that there was a strong chemical bonding between glycerol and titanium (IV) oxide, while the generated by-product was acrolein.

This research might be useful to develop the catalysts for absorption of glycerol from biofuel and conversion of glycerol into acrolein by a titanium (IV) oxide.

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