

ISSN 2518-1491 (Online),
ISSN 2224-5286 (Print)

ҚАЗАҚСТАН РЕСПУБЛИКАСЫ
ҰЛТТЫҚ ҒЫЛЫМ АКАДЕМИЯСЫНЫҢ

Д.В. Сокольский атындағы
«Жанармай, катализ және электрохимия институты» АҚ

Х А Б А Р Л А Р Ы

ИЗВЕСТИЯ

НАЦИОНАЛЬНОЙ АКАДЕМИИ НАУК
РЕСПУБЛИКИ КАЗАХСТАН
АО «Институт топлива, катализа и
электрохимии им. Д.В. Сокольского»

N E W S

OF THE ACADEMY OF SCIENCES
OF THE REPUBLIC OF KAZAKHSTAN
JSC «D.V. Sokolsky institute of fuel,
catalysis and electrochemistry»

SERIES
CHEMISTRY AND TECHNOLOGY
4 (453)

OCTOBER – DECEMBER 2022

PUBLISHED SINCE JANUARY 1947

PUBLISHED 4 TIMES A YEAR

ALMATY, NAS RK

Бас редактор:

ЖҰРЫНОВ Мұрат Жұрынұлы, химия ғылымдарының докторы, профессор, ҚР ҰҒА академигі, Қазақстан Республикасы Ұлттық ғылым академиясының президенті, АҚ «Д.В. Сокольский атындағы отын, катализ және электрохимия институтының» бас директоры (Алматы, Қазақстан) Н = 4

Редакция алқасы:

ӘДЕКЕНОВ Серғазы Мынжасарұлы (бас редактордың орынбасары), химия ғылымдарының докторы, профессор, ҚР ҰҒА академигі, «Фитохимия» Халықаралық ғылыми-өндірістік холдингінің директоры (Қарағанды, Қазақстан) Н = 11

АГАБЕКОВ Владимир Енокович (бас редактордың орынбасары), химия ғылымдарының докторы, профессор, Беларусь ҰҒА академигі, Жаңа материалдар химиясы институтының құрметті директоры (Минск, Беларусь) Н = 13

СТРНАД Мирослав, профессор, Чехия ғылым академиясының Эксперименттік ботаника институтының зертхана меңгерушісі (Оломоуц, Чехия) Н = 66

БҮРКІТБАЕВ Мұхамбетқали, химия ғылымдарының докторы, профессор, ҚР ҰҒА академигі, әл-Фараби атындағы ҚазҰУ-дың бірінші проректоры (Алматы, Қазақстан) Н = 11

ХОХМАНН Джудит, Сегед университетінің Фармацевтика факультетінің Фармакогнозия кафедрасының меңгерушісі, Жаратылыстану ғылымдарының пәнаралық орталығының директоры (Сегед, Венгрия) Н = 38

РОСС Самир, PhD докторы, Миссисипи университетінің Өсімдік өнімдерін ғылыми зерттеу ұлттық орталығы, Фармация мектебінің профессоры (Оксфорд, АҚШ) Н = 35

ХУТОРЯНСКИЙ Виталий, философия докторы (PhD, фармацевт), Реддинг университетінің профессоры (Реддинг, Англия) Н = 40

ТЕЛТАЕВ Бағдат Бұрханбайұлы, техника ғылымдарының докторы, профессор, ҚР ҰҒА корреспондент-мүшесі, Қазақстан Республикасы Индустрия және инфрақұрылымдық даму министрлігі (Алматы, Қазақстан) Н = 13

ФАРУК Асана Дар, Хамдар аль-Маджида Шығыс медицина колледжінің профессоры, Хамдард университетінің Шығыс медицина факультеті (Карачи, Пәкістан) Н = 21

ФАЗЫЛОВ Серік Драхметұлы, химия ғылымдарының докторы, профессор, ҚР ҰҒА академигі, Органикалық синтез және көмір химиясы институты директорының ғылыми жұмыстар жөніндегі орынбасары (Қарағанды, Қазақстан) Н = 6

ЖОРОБЕКОВА Шарипа Жоробекқызы, химия ғылымдарының докторы, профессор, Қырғызстан ҰҒА академигі, ҚР ҰҒА Химия және химиялық технология институты (Бішкек, Қырғызстан) Н = 4

ХАЛИКОВ Джурабай Халикович, химия ғылымдарының докторы, профессор, Тәжікстан ҒА академигі, В.И. Никитин атындағы Химия институты (Душанбе, Тәжікстан) Н = 6

ФАРЗАЛИЕВ Вагиф Меджидоглы, химия ғылымдарының докторы, профессор, ҰҒА академигі (Баку, Әзірбайжан) Н = 13

ГАРЕЛИК Хемда, философия докторы (PhD, химия), Халықаралық таза және қолданбалы химия одағының Химия және қоршаған орта бөлімінің президенті (Лондон, Англия) Н = 15

«ҚР ҰҒА Хабарлары. Химия және технология сериясы»

ISSN 2518-1491 (Online),

ISSN 2224-5286 (Print)

Меншіктенуші: «Қазақстан Республикасының Ұлттық ғылым академиясы» РҚБ (Алматы қ.). Қазақстан Республикасының Ақпарат және қоғамдық даму министрлігінің Ақпарат комитетінде 29.07.2020 ж. берілген № **KZ66VPY00025419** мерзімдік басылым тіркеуіне қойылу туралы куәлік.

Тақырыптық бағыты: *органикалық химия, бейорганикалық химия, катализ, электрохимия және коррозия, фармацевтикалық химия және технологиялар.*

Мерзімділігі: жылына 4 рет.

Тиражы: 300 дана.

Редакцияның мекен-жайы: 050010, Алматы қ., Шевченко көш., 28, 219 бөл., тел.: 272-13-19

<http://chemistry-technology.kz/index.php/en/arithv>

© Қазақстан Республикасының Ұлттық ғылым академиясы, 2022

Редакцияның мекенжайы: 050100, Алматы қ., Қонаев к-сі, 142, «Д.В. Сокольский атындағы отын, катализ және электрохимия институты» АҚ, каб. 310, тел. 291-62-80, факс 291-57-22, e-mail: orgcat@nursat.kz

Типографияның мекен-жайы: «Аруна» ЖК, Алматы қ., Мұратбаев көш., 75.

Главный редактор:

ЖУРИНОВ Мурат Журинович, доктор химических наук, профессор, академик НАН РК, президент Национальной академии наук Республики Казахстан, генеральный директор АО «Институт топлива, катализа и электрохимии им. Д.В. Сокольского» (Алматы, Казахстан) Н = 4

Редакционная коллегия:

АДЕКЕНОВ Сергазы Мынжасарович (заместитель главного редактора), доктор химических наук, профессор, академик НАН РК, директор Международного научно-производственного холдинга «Фитохимия» (Караганда, Казахстан) Н = 11

АГАБЕКОВ В ладимир Енокович (заместитель главного редактора), доктор химических наук, профессор, академик НАН Беларуси, почетный директор Института химии новых материалов (Минск, Беларусь) Н = 13

СТРНАД Мирослав, профессор, заведующий лабораторией института Экспериментальной ботаники Чешской академии наук (Оломоуц, Чехия) Н = 66

БУРКИТБАЕВ Мухамбеткали, доктор химических наук, профессор, академик НАН РК, Первый проректор КазНУ имени аль-Фараби (Алматы, Казахстан) Н = 11

ХОХМАНН Джудит, заведующий кафедрой Фармакогнозии Фармацевтического факультета Университета Сегеда, директор Междисциплинарного центра естественных наук (Сегед, Венгрия) Н = 38

РОСС Самир, доктор PhD, профессор Школы Фармации национального центра научных исследований растительных продуктов Университета Миссисипи (Оксфорд, США) Н = 35

ХУТОРЯНСКИЙ Виталий, доктор философии (Ph.D, фармацевт), профессор Университета Рединга (Рединг, Англия) Н = 40

ТЕЛЬГАЕВ Багдат Бурханбайулы, доктор технических наук, профессор, член-корреспондент НАН РК, Министерство Индустрии и инфраструктурного развития Республики Казахстан (Алматы, Казахстан) Н = 13

ФАРУК Асана Дар, профессор колледжа Восточной медицины Хамдарда аль-Маджида, факультет Восточной медицины университета Хамдарда (Карачи, Пакистан) Н = 21

ФАЗЫЛОВ Серик Драхметович, доктор химических наук, профессор, академик НАН РК, заместитель директора по научной работе Института органического синтеза и углехимии (Караганда, Казахстан) Н = 6

ЖОРОБЕКОВА Шарипа Жоробековна, доктор химических наук, профессор, академик НАН Кыргызстана, Институт химии и химической технологии НАН КР (Бишкек, Кыргызстан) Н = 4

ХАЛИКОВ Джурабай Халикович, доктор химических наук, профессор, академик АН Таджикистана, Институт химии имени В.И. Никитина АН РТ (Душанбе, Таджикистан) Н = 6

ФАРЗАЛИЕВ Вагиф Меджид оглы, доктор химических наук, профессор, академик НАНА (Баку, Азербайджан) Н = 13

ГАРЕЛИК Хемда, доктор философии (Ph.D, химия), президент Отдела химии и окружающей среды Международного союза чистой и прикладной химии (Лондон, Англия) Н = 15

«Известия НАН РК. Серия химии и технологий».

ISSN 2518-1491 (Online),

ISSN 2224-5286 (Print)

Собственник: Республиканское общественное объединение «Национальная академия наук Республики Казахстан» (г. Алматы).

Свидетельство о постановке на учет периодического печатного издания в Комитете информации Министерства информации и общественного развития Республики Казахстан № KZ66VPY00025419, выданное 29.07.2020 г.

Тематическая направленность: *органическая химия, неорганическая химия, катализ, электрохимия и коррозия, фармацевтическая химия и технологии.*

Периодичность: 4 раз в год.

Тираж: 300 экземпляров.

Адрес редакции: 050010, г. Алматы, ул. Шевченко, 28, оф. 219, тел.: 272-13-19

<http://chemistry-technology.kz/index.php/en/archiv>

© Национальная академия наук Республики Казахстан, 2022

Адрес редакции: 050100, г. Алматы, ул. Кунаева, 142, АО «Институт топлива, катализа и электрохимии им. Д.В. Сокольского», каб. 310, тел. 291-62-80, факс 291-57-22, e-mail: orgcat@nursat.kz

Адрес типографии: ИП «Аруна», г. Алматы, ул. Муратбаева, 75.

Editor in chief:

ZHURINOV Murat Zhurinovich, doctor of chemistry, professor, academician of NAS RK, president of NAS RK, general director of JSC "Institute of fuel, catalysis and electrochemistry named after D.V. Sokolsky (Almaty, Kazakhstan) H = 4

Editorial board:

ADEKENOV Sergazy Mynzhasarovich (deputy editor-in-chief) doctor of chemical sciences, professor, academician of NAS RK, director of the international Scientific and production holding «Phytochemistry» (Karaganda, Kazakhstan) H = 11

AGABEKOV Vladimir Enokovich (deputy editor-in-chief), doctor of chemistry, professor, academician of NAS of Belarus, honorary director of the Institute of Chemistry of new materials (Minsk, Belarus) H = 13

STRNAD Miroslav, head of the laboratory of the institute of Experimental Botany of the Czech academy of sciences, professor (Olomouc, Czech Republic) H = 66

BURKITBAYEV Mukhambetkali, doctor of chemistry, professor, academician of NAS RK, first vice-rector of al-Farabi KazNU (Almaty, Kazakhstan) H = 11

HOHMANN Judith, head of the department of pharmacognosy, faculty of Pharmacy, university of Szeged, director of the interdisciplinary center for Life sciences (Szeged, Hungary) H = 38

ROSS Samir, Ph.D., professor, school of Pharmacy, national center for scientific research of Herbal Products, University of Mississippi (Oxford, USA) H = 35

KHUTORYANSKY Vitaly, Ph.D., pharmacist, professor at the University of Reading (Reading, England) H = 40

TELTAYEV Bagdat Burkhanbayuly, doctor of technical sciences, professor, corresponding member of NAS RK, ministry of Industry and infrastructure development of the Republic of Kazakhstan (Almaty, Kazakhstan) H = 13

PHARUK Asana Dar, professor at Hamdard al-Majid college of Oriental medicine. faculty of Oriental medicine, Hamdard university (Karachi, Pakistan) H = 21

FAZYLOV Serik Drakhmetovich, doctor of chemistry, professor, academician of NAS RK, deputy director for institute of Organic synthesis and coal chemistry (Karaganda, Kazakhstan) H = 6

ZHOROBEKOVA Sharipa Zhorobekovna, doctor of chemistry, professor, academician of NAS of Kyrgyzstan, Institute of Chemistry and chemical technology of NAS KR (Bishkek, Kyrgyzstan) H = 4

KHALIKOV Jurabay Khalikovich, doctor of chemistry, professor, academician of the academy of sciences of Tajikistan, institute of Chemistry named after V.I. Nikitin AS RT (Tajikistan) H = 6

FARZALIEV Vagif Medzhid ogly, doctor of chemistry, professor, academician of NAS of Azerbaijan (Azerbaijan) H = 13

GARELIK Hemda, PhD in chemistry, president of the department of Chemistry and Environment of the International Union of Pure and Applied Chemistry (London, England) H = 15

News of the National Academy of Sciences of the Republic of Kazakhstan. Series of chemistry and technology.

ISSN 2518-1491 (Online),

ISSN 2224-5286 (Print)

Owner: RPA «National Academy of Sciences of the Republic of Kazakhstan» (Almaty).

The certificate of registration of a periodical printed publication in the Committee of information of the Ministry of Information and Social Development of the Republic of Kazakhstan No. **KZ66VPY00025419**, issued 29.07.2020.

Thematic scope: *organic chemistry, inorganic chemistry, catalysis, electrochemistry and corrosion, pharmaceutical chemistry and technology.*

Periodicity: 4 times a year.

Circulation: 300 copies.

Editorial address: 28, Shevchenko str., of. 219, Almaty, 050010, tel. 272-13-19

<http://chemistry-technology.kz/index.php/en/arhiv>

© National Academy of Sciences of the Republic of Kazakhstan, 2022

Editorial address: JSC «D.V. Sokolsky institute of fuel, catalysis and electrochemistry», 142, Kunayev str., of. 310, Almaty, 050100, tel. 291-62-80, fax 291-57-22, e-mail: orgcat@nursat.kz

Address of printing house: ST «Aruna», 75, Muratbayev str, Almaty.

NEWS

OF THE NATIONAL ACADEMY OF SCIENCES OF THE REPUBLIC
OF KAZAKHSTAN

SERIES CHEMISTRY AND TECHNOLOGY

<https://doi.org/10.32014/2518-1491.142>

Volume 4, Number 453 (2022) 136-144

UDC 661.74

Zh.A. Sailau^{1*}, N.Zh. Almas², K. Toshtay¹, A.A. Aldongarov³

¹Al-Farabi Kazakh National University, Almaty, Kazakhstan;

²International Science Complex Astana, Astana, Kazakhstan;

³L.N. Gumilyov Eurasian National University, Astana, Kazakhstan.
E-mail: sailau.online@gmail.com

**THEORETICAL STUDY OF THE GLYCEROL ADSORPTION FROM THE
BIOFUEL OVER TiO₂ 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.

Ж.А. Сайлау^{1*}, Н.Ж. Алмас², Қ. Тоштай¹, А.А. Алдонгаров³

¹Әл-Фараби атындағы Қазақ Ұлттық Университеті, Алматы, Қазақстан;

²Астана Халықаралық Ғылыми Кешені, Астана, Қазақстан;

³Л.Н. Гумилев атындағы Қазақ Ұлттық Евразия Университеті, Астана, Қазақстан.
E-mail: sailau.online@gmail.com

**TiO₂ КАТАЛИТИКАЛЫҚ БЕТІ АРҚЫЛЫ БИООТЫННАН
ГЛИЦЕРОЛДЫ АДСОРБЦИЯЛАУ ПРОЦЕССИН ТЕОРИЯЛЫҚ ТҮРҒЫДА
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.

Ж.А. Сайлау^{1*}, Н.Ж. Алмасов², К. Тоштай¹, А.А. Алдонгаров³

¹Казахский национальный университет имени аль-Фараби, Алматы, Казахстан;

²Международный научный комплекс Астана, Астана, Казахстан;

³Евразийский Национальный Университет имени Л.Н. Гумилева, Астана, Казахстан.

E-mail: sailau.online@gmail.com

ТЕОРЕТИЧЕСКОЕ ИССЛЕДОВАНИЕ АДСОРБЦИИ ГЛИЦЕРИНА ИЗ БИОТОПЛИВА ЧЕРЕЗ КАТАЛИТИЧЕСКУЮ ПОВЕРХНОСТЬ TiO₂

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 (Batani 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; Chakraborty 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.

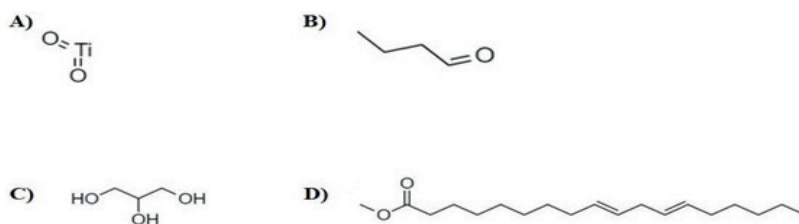


Figure 1. The 2D chemical structures of A) titanium (IV) oxide, B) acrolein, C) glycerol, and D) methyl linoleate.

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

$$E_{\text{adsorption}} = E_{(\text{TiO}_2+\text{Glycerol}+\text{Biofuel})} - (E_{(\text{Glycerol})} + E_{(\text{Biofuel})} + E_{(\text{TiO}_2)})$$

$$E_{\text{Production}} = E_{(\text{TiO}_2+\text{Acrolein}+\text{Methyl linoleate})} - (E_{(\text{Acrolein})} + E_{(\text{Biofuel})} + E_{(\text{TiO}_2)})$$

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.

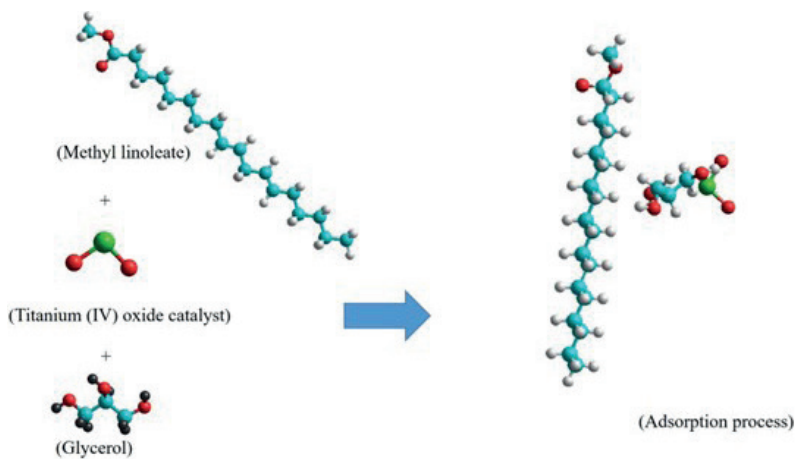


Figure 2. The electronic structures of titanium (IV) oxide, glycerol, and methyl linoleate.

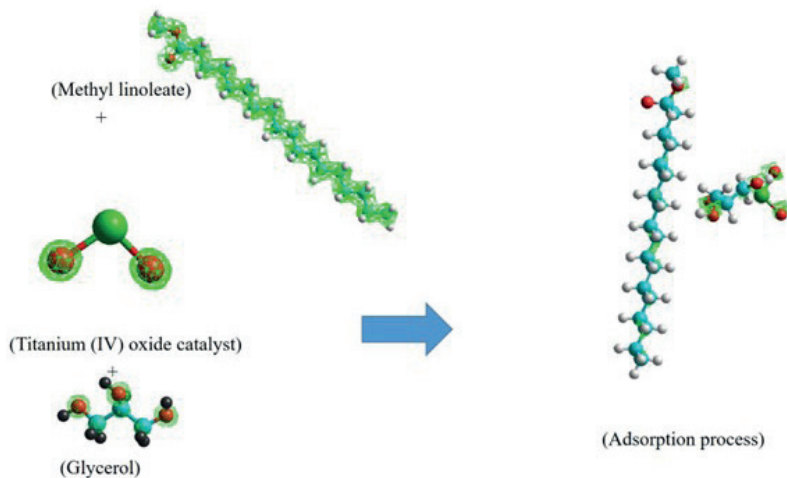


Figure 3. The molecular electrostatic maps of titanium (IV) oxide, glycerol, and methyl linoleate.

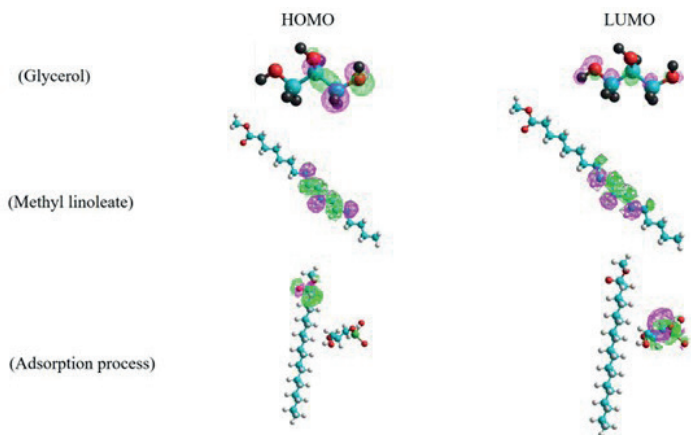


Figure 4. The molecular orbitals of titanium (IV) oxide, glycerol, and methyl linoleate.

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.

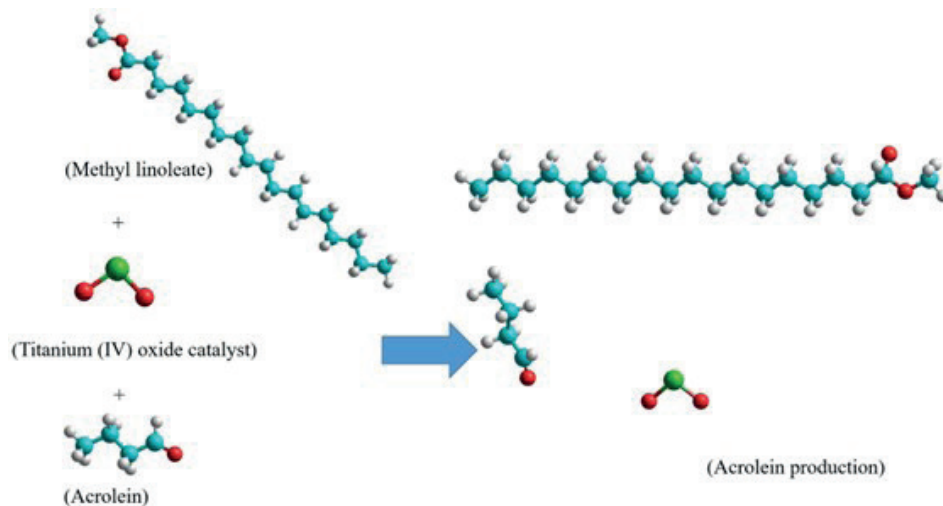


Figure 5. The electronic structures of titanium (IV) oxide, acrolein, and methyl linoleate.

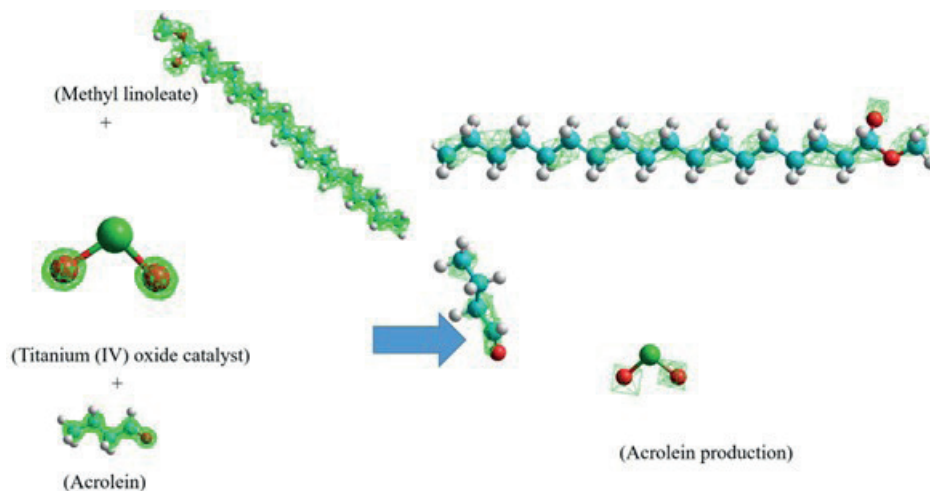


Figure 6. The molecular electrostatic maps of titanium (IV) oxide, acrolein, and methyl linoleate.

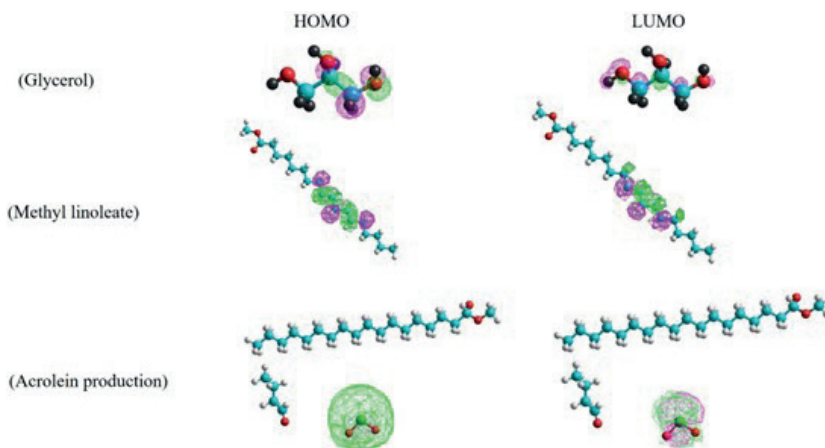


Figure 7. The molecular orbitals of titanium (IV) oxide, acrolein, and methyl linoleate.

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:

$E_{\text{adsorption}} = -126605.00 - (-31376.50 - 77595.70 - 15646) = -1986.80$ 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:

$E_{\text{production}} = -115576.00 - (- 20502.60 - 77595.70 - 15646) = -1831.70$ 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.

Information about the authors:

Sailau Zhassulan – PhD student, Department of Chemistry and Chemical Technology, Al-Farabi Kazakh National University, Almaty, Kazakhstan; sailau.online@gmail.com, Has a H-index:1 (Scopus), <https://orcid.org/0000-0001-5222-6827>;

Almas Nurlan – PhD, International Science Complex Astana, Astana, Kazakhstan; n.almas@astanait.edu.kz, Has a H-index: 1(Scopus), <https://orcid.org/0000-0003-2183-3389>;

Tostay Kainaubek – PhD, Senior Lecturer, Department of Chemistry and Chemical Technology, Al-Farabi Kazakh National University, Almaty, Kazakhstan; kainaubek.toshtay@gmail.com; <https://orcid.org/0000-0003-1182-7460>;

Aldongarov Anuar – PhD, Associated Professor, Department of Technical Physics, L.N. Gumilyov Eurasian National University, Astana, Kazakhstan; enu-2010@yandex.kz, Has a H-index:5, <https://orcid.org/0000-0001-7784-0524>.

REFERENCES

- Alonso D.M., Bond J.Q. & Dumesic J.A. (2010). Catalytic conversion of biomass to biofuels. *Green chemistry*, 12(9), 1493-1513.
- Baroutian S., Aroua M.K., Raman A.A.A., Shafie A., Ismail R.A. & Hamdan H. (2013). Blended aviation biofuel from esterified *Jatropha curcas* and waste vegetable oils. *Journal of the Taiwan Institute of Chemical Engineers*, 44(6), 911-916.
- Batani H., Saraeian A. & Able C. (2017). A comprehensive review on biodiesel purification and upgrading. *Biofuel Research Journal*, 4(3), 668-690.
- Bora P., Boro J., Konwar L.J. & Deka D. (2016). Formulation of microemulsion based hybrid biofuel

from waste cooking oil—A comparative study with biodiesel. *Journal of the Energy Institute*, 89(4), 560-568.

Chakraborty S., Nayak J., Pal P., Kumar R., Banerjee S., Mondal P.K. & Ruj B. (2020). Catalytic conversion of CO₂ to biofuel (methanol) and downstream separation in membrane-integrated photoreactor system under suitable conditions. *International Journal of Hydrogen Energy*, 45(1), 675-690.

Cheng J.J. & Timilsina G.R. (2011). Status and barriers of advanced biofuel technologies: a review. *Renewable Energy*, 36(12), 3541-3549.

Chhabra M., Saini B.S. & Dwivedi G. (2021). Impact assessment of biofuel from waste neem oil. *Energy Sources, Part A: Recovery, Utilization, and Environmental Effects*, 43(24), 3381-3392.

Crossley S., Faria J., Shen M. & Resasco D.E. (2010). Solid nanoparticles that catalyze biofuel upgrade reactions at the water/oil interface. *Science*, 327(5961), 68-72.

De Lima G.F., Mavrandonakis A., De Abreu H.A., Duarte H.A. & Heine T. (2013). Mechanism of alcohol–water separation in metal–organic frameworks. *The Journal of Physical Chemistry C*, 117(8), 4124-4130.

Ferrero G.O., Rojas H.J., Argaña C.E. & Eimer G.A. (2016). Towards sustainable biofuel production: design of a new biocatalyst to biodiesel synthesis from waste oil and commercial ethanol. *Journal of Cleaner Production*, 139, 495-503.

Gao F., Courjean O. & Mano N. (2009). An improved glucose/O₂ membrane-less biofuel cell through glucose oxidase purification. *Biosensors and Bioelectronics*, 25(2), 356-361.

Gueddida S., Lebègue S. & Badawi M. (2020). Assessing the potential of amorphous silica surfaces for the removal of phenol from biofuel: a density functional theory investigation. *The Journal of Physical Chemistry C*, 124(37), 20262-20269.

Huang X., Cheng D.G., Chen F. & Zhan X. (2016). Reaction pathways of hemicellulose and mechanism of biomass pyrolysis in hydrogen plasma: A density functional theory study. *Renewable Energy*, 96, 490-497.

Jabraoui H., Khalil I., Lebègue S. & Badawi M. (2019). Ab initio screening of cation-exchanged zeolites for biofuel purification. *Molecular Systems Design & Engineering*, 4(4), 882-892.

Khalil I., Jabraoui H., Lebègue S., Kim W.J., Aguilera L.J., Thomas K. & Badawi M. (2020). Biofuel purification: Coupling experimental and theoretical investigations for efficient separation of phenol from aromatics by zeolites. *Chemical Engineering Journal*, 402, 126264.

Lee R.A. & Lavoie J.M. (2013). From first- to third-generation biofuels: Challenges of producing a commodity from a biomass of increasing complexity. *Animal Frontiers*, 3(2), 6-11.

Li H., Fang Z., Smith Jr R.L. & Yang S. (2016). Efficient valorization of biomass to biofuels with bifunctional solid catalytic materials. *Progress in Energy and Combustion Science*, 55, 98-194.

Liang S., Liu Z., Xu M. & Zhang T. (2013). Waste oil derived biofuels in China bring brightness for global GHG mitigation. *Bioresource technology*, 131, 139-145.

Liu H., Tang X., Hao W., Zeng X., Sun Y., Lei T. & Lin L. (2018). One-pot tandem conversion of fructose into biofuel components with in-situ generated catalyst system. *Journal of Energy Chemistry*, 27(2), 375-380.

Long F., Cao X., Jiang X., Zhai Q., Zhao J., Yu S. & Xu J. (2022). An effective strategy for waste oil deoxygenation and upgrading for hydrocarbon biofuels production: A computational and experimental investigation. *Journal of the Energy Institute*, 100, 109-119.

Makoś P., Słupek E. & Gębicki J. (2020). Extractive detoxification of feedstocks for the production of biofuels using new hydrophobic deep eutectic solvents—Experimental and theoretical studies. *Journal of Molecular Liquids*, 308, 113101.

Santana J.C.C., Miranda A.C., Souza L., Yamamura C.L.K., Coelho D.D.F., Tambourgi E.B. & Ho L.L. (2021). Clean production of biofuel from waste cooking oil to reduce emissions, fuel cost, and respiratory disease hospitalizations. *Sustainability*, 13(16), 9185.

Taufiqurrahmi N., Mohamed A.R. & Bhatia S. (2011). Production of biofuel from waste cooking palm oil using nanocrystalline zeolite as catalyst: process optimization studies. *Bioresource technology*, 102(22), 10686-10694.

Yuvaraj D., Bharathiraja B., Rithika J., Dhanasree S., Ezhilarasi V., Lavanya A. & Praveenkumar R. (2019). Production of biofuels from fish wastes: an overview. *Biofuels*, 10(3), 301-307.

МАЗМҰНЫ

<p>К.Т. Бисембаева, А.С. Хадиева, Е.Н. Маммалов, Г.С. Сабырбаева, Б.М. Нуранбаева КҮРДЕЛІ ГЕОЛОГИЯЛЫҚ ЖАҒДАЙДА ПОЛИМЕРЛІК ЕРІТІНДІМЕН МҰНАЙДЫ ЫҒЫСТЫРУ ҮДЕРІСІНІҢ ЗЕРТТЕЛУІ.....</p>	5
<p>Б. Жақып, Б. Аскапова, А. Бақыт, К. Мусабеков ҚАЗАҚСТАН МОНТМОРИЛЛОНИТ НЕГІЗІНДЕ ФИЗИОЛОГИЯЛЫҚ БЕЛСЕНДІ БИОНАНОКОМПОЗИТТЕРДІ АЛУ.....</p>	14
<p>М. Жумабек, С.А. Тунгатарова, Г.Н. Кауменова, А. Манабаева, С.О. Котов ТАБИҒИ ГАЗДЫ КОМПОЗИТТИ Ni-Co-Zr КАТАЛИЗАТОРЛАРЫНДА ПАРЦИАЛДЫ ТОТЫҚТЫРУ.....</p>	26
<p>Ш.С. Ислам, Х.С. Рафиқова, С.Б. Рыспаева, А.Ж. Керімқұлова, М.А. Кожайсақова МОТОР ОТЫНЫНАН КҮКІРТ ҚОСЫЛЫСТАРЫН ТЕРЕҢ ЭВТЕКТИКАЛЫҚ ЕРІТКІШТЕРМЕН БӨЛІП АЛУ.....</p>	37
<p>Г.Н. Калматаева, Г.Ф. Сагитова, С.А. Сакибаева, Д.Д. Асылбекова, Ж.К. Шуханова ШИНА РЕГЕНЕРАТЫ ӨНДІРІСІНДЕ МАЙ ӨНЕРКӘСІБІНІҢ ІЛЕСПЕ ӨНІМДЕРІН ПАЙДАЛАҢУ.....</p>	46
<p>Ж. Касенова, С. Кожабеков, Ә. Жубанов, А. Ғалымжан АЛКИЛ ФУМАРАТТАР МЕН ОКТАДЕЦЕН-1-НІҢ СОПОЛИМЕРЛЕРІН СИНТЕЗДЕУ ЖӘНЕ ЗЕРТТЕУ.....</p>	58
<p>Р.М. Қудайбергенова, Н.С. Мурзакасымова, С.М. Кантарбаева, Д.Т. Алтынбекова, Г.К. Сугурбекова ГРАФЕН, ГО, ТГО РАМАНДЫҚ СПЕКТРОСКОПИЯСЫ.....</p>	69
<p>А. Қадырбаева, Д. Уразкелдиева, Р. Тәңірбергенов, Г. Шаймерденова ҚАЗАҚСТАН РЕСПУБЛИКАСЫНДАҒЫ «ТАСТЫ ТҰЗ» КЕН ОРНЫНДАҒЫ ТЕХНИКАЛЫҚ НАТРИЙ ХЛОРИДІН ТАЗАЛАУ.....</p>	80
<p>Ж.Н. Қорғанбеков, А.А. Өтебаев, Р.М. Мухамедов «ТОПЫРАҚ-ӨСІМДІК» ЖҮЙЕСІНДЕ АУЫР МЕТАЛДАРДЫҢ ЖИНАЛУЫ ЖӘНЕ ТАРАЛУЫ.....</p>	88
<p>К.М. Маханбетова, Э.К. Асембаева, Д.Е. Нурмуханбетова, Е.Ж. Габдуллина, М. Ілиясқызы ЕШКІ СҮТІ – БИОЛОГИЯЛЫҚ ТОЛЫҚҚҰНДЫ ШИКІЗАТ.....</p>	96

Б.Ж. Мулдабекова, А.М. Токтарова, Р.А. Изтелиева, М.Б. Атыханова, А. А. Сейдімханова КОМПОЗИТТІК ҰНДАРДЫҢ САПАСЫ МЕН ҚАУІПСІЗДІГІН БАҚЫЛАУ.....	107
Н.С. Мурзакасымова, М.А. Гавриленко, Н.А. Бектенов, Р.М. Кудайбергенова, Г.А. Сейтбекова МОДИФИКАЦИЯЛАНҒАН КӨМІРДЕ АУЫР МЕТАЛДАРДЫҢ СОРБЦИЯСЫН ЗЕРТТЕУ.....	118
А.А. Өтебаев, Ж.Н. Қорғанбеков, Р.М. Мухамедов КӨКӨНІС ДАҚЫЛДАРЫНДАҒЫ АУЫР МЕТЕЛДАРДЫ БИОТЕСТІЛЕУ.....	126
Ж.А. Сайлау, Н.Ж. Алмас, Қ. Тоштай, А.А. Алдонгаров TiO ₂ КАТАЛИТИКАЛЫҚ БЕТІ АРҚЫЛЫ БИООТЫННАН ГЛИЦЕРОЛДЫ АДСОРБЦИЯЛАУ ПРОЦЕССИН ТЕОРИЯЛЫҚ ТҰРҒЫДА ЗЕРТТЕУ.....	136

СОДЕРЖАНИЕ

К.Т. Бисембаева, А.С. Хадиева, Е.Н. Маммалов, Г.С. Сабырбаева, Б.М. Нуранбаева ИССЛЕДОВАНИЕ ПРОЦЕССА ВЫТЕСНЕНИЯ НЕФТИ ПОЛИМЕРНЫМИ РАСТВОРАМИ В СЛОЖНЫХ ГЕОЛОГИЧЕСКИХ УСЛОВИЯХ.....	5
Б. Жақып, Б. Аскапова, А. Бақыт, К. Мусабеков РАЗРАБОТКА ФИЗИОЛОГИЧЕСКИ АКТИВНЫХ БИОНАНОКОМПОЗИТОВ НА ОСНОВЕ КАЗАХСТАНСКОГО МОНТМОРИЛЛОНИТА.....	14
М. Жумабек, С.А. Тунгатарова, Г.Н. Кауменова, А. Манабаева, С.О. Котов Ni-Co-Zr КОМПОЗИТНЫЕ КАТАЛИЗАТОРЫ ПАРЦИАЛЬНОГО ОКИСЛЕНИЯ ПРИРОДНОГО ГАЗА.....	26
Ш.С. Ислам, Х.С. Рафикова, С.Б. Рыспаева, А.Ж. Керимкулова, М.А. Кожайсакова ИЗВЛЕЧЕНИЕ СОЕДИНЕНИЙ СЕРЫ ИЗ МОТОРНОГО ТОПЛИВА ГЛУБОКИМИ ЭВТЕКТИЧЕСКИМИ РАСТВОРИТЕЛЯМИ.....	37
Г.Н. Калматаева, Г.Ф. Сагитова, С.А. Сакибаева, Д.Д. Асылбекова, Ж.К. Шуханова ИСПОЛЬЗОВАНИЕ СОПУТСТВУЮЩИХ ПРОДУКТОВ МАСЛОЖИРОВОЙ ПРОМЫШЛЕННОСТИ В ПРОИЗВОДСТВЕ ШИННОГО РЕГЕНЕРАТА.....	46
Ж. Касенова, С. Кожабеков, Э. Жубанов, А. Галымжан СИНТЕЗ И ИССЛЕДОВАНИЕ ГРЕБНЕОБРАЗНЫХ СОПОЛИМЕРОВ АЛКИЛ ФУМАРАТОВ С ОКТАДЕЦЕНОМ-1.....	58
Р.М. Кудайбергенова, Н.С. Мурзакасымова, С.М. Кантарбаева, Д.Т. Алтынбекова, Г.К. Сугурбекова РАМАНОВСКАЯ СПЕКТРОСКОПИЯ ГРАФЕНА, ГО, ВГО.....	69
А. Кадырбаева, Д. Уразкелдиева, Р. Танирбергенов, Г. Шаймерденова ОЧИСТКА ТЕХНИЧЕСКОГО ХЛОРИДА НАТРИЯ МЕСТОРОЖДЕНИЯ «ТАСТЫ ТҮЗ» РЕСПУБЛИКИ КАЗАХСТАН.....	80
Ж.Н. Курганбеков, А.А. Утебаев, Р.С. Мухамедов НАКОПЛЕНИЕ И РАСПРЕДЕЛЕНИЕ ТЯЖЕЛЫХ МЕТАЛЛОВ В СИСТЕМЕ «ПОЧВА-РАСТЕНИЕ».....	88

- К.М. Маханбетова, Э.К. Асембаева, Д.Е. Нурмуханбетова, Е.Ж. Габдуллина,
М. Илияскызы**
КОЗЬЕ МОЛОКО – ПОЛНОЦЕННОЕ БИОЛОГИЧЕСКОЕ СЫРЬЕ.....96
- Б.Ж. Мулдабекова, А.М. Токтарова, Р.А. Изтелиева, М.Б. Атыханова,
А.А. Сейдімханова**
КОНТРОЛЬ КАЧЕСТВА И БЕЗОПАСНОСТИ КОМПОЗИТНОЙ МУКИ.....107
- Н.С. Мурзакасымова, М.А. Гавриленко, Н.А. Бектенов,
Р.М. Кудайбергенова, Г.А. Сейтбекова**
ИССЛЕДОВАНИЕ СОРБЦИИ ТЯЖЕЛЫХ МЕТАЛЛОВ
НА МОДИФИЦИРОВАННОМ УГЛЕ.....118
- А.А.Утебаев, Ж.Н.Курганбеков, Р.С.Мухамедов**
БИОТЕСТИРОВАНИЕ ТЯЖЕЛЫХ МЕТАЛЛОВ В ОВОЩНЫХ
КУЛЬТУРАХ.....126
- Ж.А. Сайлау, Н.Ж. Алмасов, К. Тоштай, А.А. Алдонгаров**
ТЕОРЕТИЧЕСКОЕ ИССЛЕДОВАНИЕ АДСОРБЦИИ ГЛИЦЕРИНА
ИЗ БИОТОПЛИВА ЧЕРЕЗ КАТАЛИТИЧЕСКУЮ ПОВЕРХНОСТЬ TiO_2136

CONTENTS

K. Bissembayeva, A. Khadiyeva, E. Mamalov, G. Sabyrbayeva, B. Nuranbayeva
RESEARCH OF THE PROCESS OF OIL DISPLACEMENT BY POLYMER
SOLUTION IN COMPLICATED GEOLOGICAL CONDITIONS.....5

B. Zhakyp, B. Askapova, A. Bakyt, K. Musabekov
DEVELOPMENT OF PHYSIOLOGICALLY ACTIVE BIONANOCOMPOSITES
BASED ON KAZAKHSTAN MONTMORILLONITE.....14

M. Zhumabek, S.A. Tungatarova, G.N. Kaumenova, A. Manabayeva, S.O. Kotov
Ni-Co-Zr COMPOSITE CATALYSTS FOR PARTIAL OXIDATION
OF NATURAL GAS.....26

**Sh.S. Islam, Kh.S. Rafikova, S.B. Ryspaeva, A.Zh. Kerimkulova,
M.A. Kozhaisakova**
EXTRACTION OF SULFUR COMPOUNDS FROM MOTOR FUEL WITH
DEEP EUTECTIC SOLVENTS.....37

**G.N. Kalamatayeva, G.F. Sagitova, S.A. Sakibayeva, D.D. Asylbekova,
Zh.K. Shukhanova**
THE USE OF RELATED PRODUCTS OF THE FAT AND OIL INDUSTRY
IN THE PRODUCTION OF TIRE REGENERATE.....46

Zh. Kassenova, S. Kozhabekov, A. Zhubanov, A. Galymzhan
SYNTHESIS AND CHARACTERIZATION OF COMB-LIKE ALKYL
FUMARATE – OCTADECEN-1 COPOLYMERS.....58

**R. Kudaibergenova, N. Murzakassymova, S. Kantarbaeva, D. Altynbekova,
G. Sugurbekova**
RAMAN SPECTROSCOPY OF GRAPHENE, GO, RGO.....69

A. Kadirbayeva, D. Urazkeldiyeva, R. Tanirbergenov, G. Shaimerdenova
PURIFICATION OF TECHNICAL SODIUM CHLORIDE FROM THE TASTY
TUZ DEPOSIT OF THE REPUBLIC OF KAZAKHSTAN.....80

ZH.N. Kurganbekov, A.A. Utebaev, R.S. Muhamedov
ACCUMULATION AND DISTRIBUTION OF HEAVY METALS IN THE
SOIL-PLANT SYSTEM.....88

**K.M. Makhanbetova, E.K. Assembayeva, D.E. Nurmukhanbetova,
E.Zh. Gabdullina, M. Iliyaskyzy**
GOAT'S MILK – WHOLE BIOLOGICAL RAW MATERIAL.....96

B. Muldabekova, A. Toktarova, R. Iztelieva, M. Atykhanova, A. Seidimkhanova
QUALITY AND SAFETY CONTROL OF COMPOSITE FLOUR.....107

**N.S. Murzakassymova, M.A. Gavrilenko, N.A. Bektenov, R.M.Kudaibergenova,
G.A. Seitbekova¹**
INVESTIGATION OF THE SORPTION OF HEAVY METALS
ON MODIFIED COAL.....118

A.A. Utebaev, Zh.N. Kurganbekov, R.S. Muhamedov
BIOTESTING OF HEAVY METALS IN VEGETABLE CROPS.....126

Zh.A. Sailau, N.Zh. Almas, K. Toshtay, A.A. Aldongarov
THEORETICAL STUDY OF THE GLYCEROL ADSORPTION FROM
THE BIOFUEL OVER TiO₂ CATALYTIC SURFACE.....136

Publication Ethics and Publication Malpractice in the journals of the National Academy of Sciences of the Republic of Kazakhstan

For information on Ethics in publishing and Ethical guidelines for journal publication see <http://www.elsevier.com/publishingethics> and <http://www.elsevier.com/journal-authors/ethics>.

Submission of an article to the National Academy of Sciences of the Republic of Kazakhstan implies that the described work has not been published previously (except in the form of an abstract or as part of a published lecture or academic thesis or as an electronic preprint, see <http://www.elsevier.com/postingpolicy>), that it is not under consideration for publication elsewhere, that its publication is approved by all authors and tacitly or explicitly by the responsible authorities where the work was carried out, and that, if accepted, it will not be published elsewhere in the same form, in English or in any other language, including electronically without the written consent of the copyright-holder. In particular, translations into English of papers already published in another language are not accepted.

No other forms of scientific misconduct are allowed, such as plagiarism, falsification, fraudulent data, incorrect interpretation of other works, incorrect citations, etc. The National Academy of Sciences of the Republic of Kazakhstan follows the Code of Conduct of the Committee on Publication Ethics (COPE), and follows the COPE Flowcharts for Resolving Cases of Suspected Misconduct (http://publicationethics.org/files/u2/New_Code.pdf). To verify originality, your article may be checked by the Cross Check originality detection service <http://www.elsevier.com/editors/plagdetect>.

The authors are obliged to participate in peer review process and be ready to provide corrections, clarifications, retractions and apologies when needed. All authors of a paper should have significantly contributed to the research.

The reviewers should provide objective judgments and should point out relevant published works which are not yet cited. Reviewed articles should be treated confidentially. The reviewers will be chosen in such a way that there is no conflict of interests with respect to the research, the authors and/or the research funders.

The editors have complete responsibility and authority to reject or accept a paper, and they will only accept a paper when reasonably certain. They will preserve anonymity of reviewers and promote publication of corrections, clarifications, retractions and apologies when needed. The acceptance of a paper automatically implies the copyright transfer to the National Academy of Sciences of the Republic of Kazakhstan.

The Editorial Board of the National Academy of Sciences of the Republic of Kazakhstan will monitor and safeguard publishing ethics.

Правила оформления статьи для публикации в журнале смотреть на сайте:

www.nauka-nanrk.kz

<http://chemistry-technology.kz/index.php/en/arhiv>

ISSN 2518-1491 (Online), ISSN 2224-5286 (Print)

Директор отдела издания научных журналов НАН РК *А. Ботанқызы*
Заместитель директор отдела издания научных журналов НАН РК *Р. Жәліқызы*

Редакторы: *М.С. Ахметова, Д.С. Аленов*

Верстка на компьютере *Г.Д. Жадырановой*

Подписано в печать 05.12.2022.

Формат 60x88¹/₈. Бумага офсетная. Печать – ризограф.

9,0 п.л. Тираж 300. Заказ 4.