

chemical approaches, have been proposed to convert GO to an electrical conductor.

In our group, we use the local thermal effect in the form of high power laser irradiation to remove the structural oxygen groups and control electrical conductivity. This way we also perform patterning with the desired geometry, contrary to the cases of other methods [1].

However, GO also is suffering from several disadvantages. Harsh oxidation produces vacancy defects that could not be removed completely following any reduction pattern [2]. What is more important, mechanical robustness of rGO on flexible substrates is insufficient, which limits its applications in sensors and wearables. Hereby we propose a green, scalable and easy-to-perform method of synthesis of graphene functionalized with aromatic compounds (ModG). We developed a way of bulk graphite electrochemical exfoliation with simultaneous diazonium functionalization. ModG demonstrates highly hydrophilic behavior and could be used as a GO alternative in terms of films fabrication on multiple substrates, including flexible ones.

In the same way, as for GO, we used a laser irradiation approach to remove aryl functionalization.

Noticeably, resulting material (LModG) demonstrates higher conductivity values compared to rGO prepared under the same conditions [3].

We performed a full characterization of ModG and LModG films on glass and polymer substrates. Contact angle experiment results indicated a drastic change in wettability after laser treatment, which indirectly demonstrates a successful removal of functional groups, which was also proved using IR spectroscopy. X-ray diffraction and Raman spectroscopy showed a high ModG crystallinity. Atomic force microscopy showed a thickness and conductivity of single layers.

An especially important finding is that ModG laser treatment on polyethylene terephthalate (PET) leads to the fabrication of not only conductive but highly mechanically robust structures. X-ray photoelectron spectroscopy data prove our theory that local temperature treatment leads to a formation of LModG/PET composite structure. Therefore this water and scratch-resistant material shows a high potential for the use in flexible electronics.

For now, LModG was used for the fabrication of chemical, electrochemical, skin conductance and bending sensors.

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## ASSESSMENT THE THERMODYNAMIC PROBABILITY OF AROMATIC HYDROCARBON FORMATION REACTIONS OCCURRENCE UNDER THE CONDITIONS OF n-HEXANE ZEOFORMING

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Production of high environmental classes motor fuel components requires to reduce the content of aromatic hydrocarbons in them and increase the

content of hydrocarbons with isostructure, which also increase the octane number of fuel.

This effect can be achieved by the use of zeolite catalysts containing acidic active centers which accelerate the isomerization reactions, and capable prevent aromatization reactions in non-standard process conditions [1]. For the production of high-octane components of gasoline with a low content of aromatic hydrocarbons Zeoforming process is used.

The major proportion of aromatic hydrocarbons in the products of Zeoforming process is benzene, toluene and xylene.

Therefore, the aim of this work is assessment the thermodynamic probability of aromatic hydro-

carbon formation reactions occurrence under the conditions of n-hexane zeoforming.

Formation of aromatic hydrocarbons by hydrogen transfer reactions in olefins, which formed during cracking is typical for Zeoforming process.

Using software Gaussian package (Gaussian-View 3.0) [2] thermodynamic characteristics (TDC) of substances and their formation reactions were calculated.

The calculation was carried out for reactions of benzene, toluene, and xylene formation, by hydrogen transfer reactions in olefins under conditions of process Zeoforming realization – temperature

**Table 1.** TDC of some reactions with benzene

№	Reaction	$\Delta H$ , kJ/mol	$\Delta S$ , kJ/mol·K	$\Delta G$ , kJ/mol
1	2 penten = benzene + ethane + 2 methane	-126.73	165.66	-234.08
2	penten + ethene + propen = benzene + ethane + 2 methane	-222.00	40.01	-247.93
3	penten + 2 propen = benzene + 2 ethane + methane	-202.23	33.24	-223.76
4	penten + 3 ethene = benzene + propane + 2 methane	-330.93	-63.41	-289.85
5	penten + propen + butene = benzene + 3 ethane	-196.16	39.92	-222.03
6	penten + 2 ethene + propen = benzene + butane + 2 methane	-318.19	-77.39	-268.04
7	2 penten + propen = benzene + 2 ethane + propen	-196.12	48.69	-227.67
8	penten + 4 ethene = benzene + 2 propane + methane	-420.10	-173.60	-307.60
9	penten + 3 propen = benzene + butane + 2 ethane	-278.64	-90.94	-219.71
10	penten + 3 ethene + propen = benzene + butane + propane + methane	-407.35	-187.59	-285.79
11	penten + 2 propen + butene = benzene + hexane + ethane + methane	-286.14	-99.34	-221.77
12	penten + 5 ethene = benzene + 3 propane	-509.26	-283.80	-325.35
13	2 penten + 2 propen = benzene + hexane + 2 ethane	-278.89	-91.53	-219.58
14	penten + 4 ethene + propen = benzene + butane + 2 propane	-496.51	-297.79	-303.55

**Table 2.** TDC of some reactions with toluene

№	Reaction	$\Delta H$ , kJ/mol	$\Delta S$ , kJ/mol·K	$\Delta G$ , kJ/mol
1	2 penten = toluene + 3 methane	-141.08	175.40	-254.74
2	penten + propen + ethene = toluene + 3 methane	-236.35	49.76	-268.59
3	penten + 2 propen = toluene + ethane + 2 methane	-216.58	42.98	-244.43
4	penten + 3 ethene = toluene + ethane + 2 methane	-338.08	-54.63	-302.68
5	penten + butene + propen = toluene + 2 ethane + methane	-210.51	49.66	-242.69
6	penten + propen + 2 butene = toluene + propane + 2 methane	-325.51	-60.44	-286.34
7	2 penten + propen = toluene + 3 ethane	-203.26	57.47	-240.50
8	penten + 4 ethene = toluene + butane + 2 methane	-434.27	-172.03	-322.79
9	penten + 3 propen = toluene + butane + ethane + ethane	-292.99	-81.20	-240.38
10	penten + propen + 3 ethene = toluene + 2 propane + ethane	-414.67	-170.64	-304.10
11	penten + butene + 2 propen = toluene + butane + 2 ethane	-286.93	-74.52	-238.64
12	penten + 5 ethene = toluene + butane + propane + ethane	-523.43	-282.23	-340.55
13	2 penten + 2 propen = toluene + hexane + ethane + methane	-293.24	-81.79	-240.24
14	penten + propen + 4 ethene = toluene + 3 propane	-503.83	-280.83	-381.85

**Table 3.** TDC of some reactions with o-xylene

№	Reaction	$\Delta H$ , kJ/mol	$\Delta S$ , kJ/mol·K	$\Delta G$ , kJ/mol
1	penten + 2 propen = o-xylene + 3 methane	-230.62	22.00	-244.88
2	penten + 3 ethene = o-xylene + 3 methane	-352.12	-75.60	-303.13
3	penten + propen + butene = o-xylene + ethane + 2 methane	-224.56	28.68	-243.14
4	penten + 2 ethene + propen = o-xylene + ethane + 2 methane	-332.35	-82.38	-278.97
5	2 penten + propen = o-xylene + 2 ethane + methane	-217.31	36.49	-240.95
6	penten + 4 ethene = o-xylene + propane + 2 methane	-441.21	-185.80	-320.89
7	penten + 3 propen = o-xylene + 3 ethane	-292.8	-95.93	-230.64
8	penten + 3 ethene + propen = o-xylene + butane + 2 methane	-428.54	-199.79	-299.08
9	penten + 2 propen + butene = o-xylene + propane + 2 ethane	-293.94	-88.29	-236.73
10	penten + 5 ethene = o-xylene + pentane + 2 methane	-536.83	-307.05	-337.86
11	2 penten + 2 propen = o-xylene + butane + 2 ethane	-293.73	-87.69	-236.90
12	penten + 4 ethene + propen = o-xylene + butane + propane + methane	-517.70	-309.98	-316.83

375 °C (648 K) and a pressure of 25 atm. (2.5 MPa). Tables 1–3 show list of some received reactions and their TDC.

The obtained results show that the flow of all the reactions is thermodynamically possible ( $\Delta G < 0$ ).

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## UPGRADING ON ZEOLITE – EFFECTIVE WAY TO OBTAIN LOW COLD-TEST DIESEL FUELS

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Despite the increase in diesel fuel production in 2018 to 77.5 million tons (an increase of 0.6 million tons compared to 2017), the share of the diesel fuel of Arctic brand in the production structure does not exceed 5% [1]

Today, the most common method for improving the low-temperature properties of fuels is using of depressant additives, but this method is not universal, since the effectiveness of the additive depends on the composition of the fuel [2].

An alternative method is the catalytic dewaxing process. However, applying a catalyst containing noble metals and a hydrogen-containing gas in this process limits the implementation of the process at

small-scale oil refineries. Therefore, it seems promising to develop processes for the upgrading of diesel fractions on zeolite catalysts, without using of hydrogen-containing gas.

The authors of the work carried out the process of upgrading straight-run diesel fraction on a laboratory catalytic unit, using a KN-30 brand zeolite catalyst. The process was carried out at the following technological parameters: process temperature – 375 °C, pressure – 0.35 MPa, feedstock speed velocity – 0.5 ml/min.

The aim of the work is studying the group hydrocarbon composition, low-temperature and physicochemical properties of the raw straight-run diesel