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Investigation of the Adsorption Properties of Electrically Conductive Pyrolyzed Polyacrylonitrile Modified with Chromium (III) Oxide to Obtain Highly Efficient Gas Sensors

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Abstract

Introduction. Obtaining highly sensitive gas sensors is an urgent task, the solution to which will allow you to accurately and quickly assess changes in the air-gas composition of a given medium. Gas sensors based on metal-containing pyrolyzed polyacrylonitriles (Me-pPAN) are among the cheapest and most environmentally friendly gas-sensitive materials with a fast response. One of the types of sensor materials included in the Me-pPAN list is pyrolyzed polyacrylonitrile (pPAN) modified with a chromium (III) oxide molecule. The reasons for selective adsorption of pPAN and Me-pPAN to pollutant gases, which would allow controlling this process and obtaining sensory materials with increased sensitivity to gases, are not enough studied. Therefore, the aim of this work was to establish the main causes of selective adsorption of semiconductor electrically conductive films by modeling methods in the framework of molecular and quantum mechanics.

Materials and Methods. The authors used modeling methods in the framework of molecular and quantum mechanics (MM2), the density functional theory (COSMO) method and the semi-empirical PM7 method in the MOPAC software package.

Results. MM2 and PM7 methods were used to obtain models of adsorption complexes of "Cr-pPAN – gas-pollutant" systems. Thermodynamic parameters of the system were calculated for standard environmental conditions. The dependence of the adsorption of pollutant gases on the surface of Cr-pPAN on temperature has been established.

Discussion and Conclusion. As a result of calculating the thermodynamic parameters of gas-pollutant–pPAN/Me-pPAN systems and obtaining positive values of Gibbs energies of these systems, it was confirmed that the adsorption of polluting gases on the surface of Cr-pPAN was not a spontaneous phenomenon and was effective at high temperatures. Considering that when chromium (III) oxide was introduced into the pPAN matrix, the charge on nitrogen atoms increased. It could be concluded that a chromium (III) oxide molecule had a positive effect on the semiconductor properties of pPAN. It was found that the adsorption of polluting gases (SO_2 and NO_2) was most likely on the surfaces of pPAN and Cr-pPAN. The results obtained in the work can be used to obtain gas-sensitive materials with specified metrological characteristics.

Keywords: pyrolyzed polyacrylonitrile (pPAN), chromium-containing polyacrylonitrile, quantum chemical model, molecular modeling, adsorption of pollutant gases, semi-empirical method, electron density, thermodynamics of the adsorption process

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Научная статья

Исследование адсорбционных свойств электропроводящего пиролизованного полиакрилонитрила, модифицированного оксидом хрома (III), для получения высокоэффективных сенсоров газов

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Аннотация

Введение. Получение высокочувствительных сенсоров газа является актуальной задачей, решение которой позволит точно и быстро оценивать изменения в воздушно-газовом составе заданной среды. К наиболее дешевым и экологичным газочувствительным материалам, отличающимся быстрым откликом, относятся сенсоры газов на основе металлсодержащих пиролизованных полиакрилонитрилов (Me-пПАН). Одним из видов сенсорных материалов, входящих в перечень Me-пПАН, является пиролизованный полиакрилонитрил (пПАН), модифицированный молекулой оксида хрома (III). Причины селективной адсорбции у пПАН и у Me-пПАН к газам-поллютантам, которые позволили бы управлять данным процессом и получать сенсорные материалы с повышенной чувствительностью к газам, в настоящее время не изучены. Поэтому целью данной работы было установление основных причин селективной адсорбции полупроводниковых электропроводящих пленок методами моделирования в рамках молекулярной и квантовой механики.

Материалы и методы. Использовались методы моделирования в рамках молекулярной и квантовой механики (ММ2), метод теории функционала плотности (COSMO) и полуэмпирический PM7-метод в программном пакете MOPAC.

Результаты исследования. Методами ММ2 и PM7 получены модели адсорбционных комплексов систем «Cr-пПАН — газ-загрязнитель». Рассчитаны термодинамические параметры системы для стандартных условий окружающей среды. Установлена зависимость адсорбции газов-загрязнителей на поверхности Cr-пПАН от температуры.

Обсуждение и заключение. В результате расчета термодинамических показателей систем «газ-загрязнителель — пПАН/Me-пПАН» и получения положительных значений величин энергий Гиббса данных систем потверждено, что адсорбция газов-загрязнителей на поверхности Cr-пПАН не является спонтанным и самопроизвольным явлением и эффективна при высоких температурах. Учитывая, что при внедрении оксида хрома (III) в матрицу пПАН, происходит увеличение заряда на атомах азота, можно сделать вывод о положительном влиянии молекулы оксида хрома (III) на полупроводниковые свойства пПАН. Установлено, что на поверхностях пПАН и Cr-пПАН наиболее вероятна адсорбция газов-загрязнителей (SO_2 и NO_2). Результаты, полученные в работе, можно использовать для получения газочувствительных материалов с заданными метрологическими характеристиками.

Ключевые слова: пиролизованный полиакрилонитрил (пПАН), хромсодержащий полиакрилонитрил, квантово-химическая модель, молекулярное моделирование, адсорбция газов-загрязнителей, полуэмпирический метод, электронная плотность, термодинамика процесса адсорбции

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Introduction. Rapid monitoring of changes in the air mixture composition in the atmospheric air and in the working area of an industrial enterprise is a necessary measure to assess the impact of production activities on the environment. For these purposes, resistive gas sensors based on modified nanocomposite semiconductor materials are used [1–7]. Gas sensors based on metal-containing pyrolyzed polyacrylonitriles (Me-pPAN) are the cheapest and most environmentally friendly. They are characterized by a rapid response to the presence of pollutants in the air mixture (NO_2, Cl_2, H_2S, CO) among sensor devices [8–11].

In [12–16], to determine the causes of selective adsorption of polluting gases on the surface of pyrolyzed polyacrylonitrile (pPAN) modified with metal oxides, contact processes were simulated using quantum and molecular mechanics methods. In the course of the conducted studies, it was found that one of the promising gas-sensitive materials was pPAN modified with chromium additives (Cr-pPAN) [17]. The fundamental reason for the use of this material was the registration of high indicators of electrical conductivity, more than nine times higher than those for unmodified pPAN [11, 12].

Studies [11, 17], showed that the Cr-modified pPAN surface had a unique feature and selectivity of adsorption with respect to NO_2, Cl_2 and NH_3 under standard environmental conditions. In order to determine the causes of selective gas sensitivity in Cr-pPan, studies were conducted using quantum and molecular mechanics methods [17]. As a result of the research, it was determined that during the adsorption of the pollutant gas on the surface of the sensor-Cr-pPAN, a Van der Waals interaction occurred between the components of the system at the level of 3.5Å-5Å.

According to [18, 19], it is known that the presence of a modifying additive in pPAN contributes to an increase in its semiconductor properties, which was demonstrated in previously published works. According to [17], COSMO method within the framework of the density functional theory confirmed that the introduction of chromium (III) oxide molecules into the pPAN structure led to an increase in semiconductor properties.

Thin-film material based on Cr-pPAN was obtained as a result of polymerization of chromocarbonyl PAN at IR annealing temperatures from 200°C to 400°C [7]. Based on the data of X-ray emission spectroscopy [11], Cr-pPAN films were a pPAN matrix with a chromium (III) oxide molecule embedded in the interplanar spacing.

In previous works [12-17] devoted to the study of the interaction of pollutant gases with the surface of Cr-pPAN, the influence of environmental conditions on adsorption processes was not taken into account. Currently, the causes of selective adsorption of pPAN and Me-pPAN to pollutants, which would allow controlling this process and obtaining sensory materials with increased sensitivity to gases, have not been studied. In addition, an important task is to evaluate the efficiency of the adsorption of polluting gases on the surface of Cr-pPAN under various temperature conditions, the choice of conditions that ensure the most beneficial interaction of components in the "Cr-pPAN – gas-pollutant" system. Therefore, the aim of this work was to determine the main causes of selective adsorption in semiconductor electrically conductive films by modeling methods in the framework of molecular and quantum mechanics, as well as to study the formation process of pPAN modified by a chromium (III) oxide molecule within the framework of the density functional theory. Within the framework of this aim, the main objective of the study for obtaining highly efficient gas sensors was to study the adsorption properties of electrically conductive pyrolyzed polyacrylonitrile modified with chromium (III) oxide.

Materials and Methods. Calculation of thermodynamic parameters of the process of interaction of pollutant gases with Cr-pPAN was carried out using a semi-empirical method within the framework of the MOPAC program.

In the framework of the MM2 method, the energetically advantageous configurations of the initial compounds — chromium (III) oxide in the pPAN matrix, the unmodified pPAN model were obtained. The adsorption complexes (AC) "Cr-pPAN – gas-pollutant" were modeled and the interaction energies were calculated (Fig. 1). Then, in order to predict the adsorption of gases-pollutants (H_2S, NH_3, CH_4, CO_2, NO_2, SO_2, O_3, CO, Cl_2) on the Cr-pPAN surface, thermodynamic parameters of the process were calculated by the semi-empirical PM7 method in the MOPAC program.

When implementing the calculations, the initial structures and models of the "Cr-pPAN – gas-pollutant" adsorption complexes were subjected to preliminary optimization by the method of coordinate descent. At this stage of modeling, the distances from the extreme atom of the adsorbate molecule to the nearest atom of the adsorbent, the modified and/or unmodified pPAN surface, were estimated.

The PM7 method was used to evaluate the spontaneity of interaction and the efficiency of adsorption of pollutant gases on the surface of unmodified pPAN and on the modified surface of Cr-pPAN.

At each stage we calculated the thermodynamic parameters (ΔH, ΔS, ΔG) of the processes at a temperature of 298K according to the following formulas:

$$\Delta H_{\text{adsorbtion}} = \Delta H_{\text{AKC}} - \left(\Delta H_{\text{gas}} + \Delta H_{\text{surface}}\right)$$

$$\Delta S_{\text{adsorbtion}} = \Delta S_{\text{AKC}} - \left(\Delta S_{\text{gas}} + \Delta S_{\text{surface}}\right)$$

$$\Delta G_{\text{adsorbtion}} = \Delta H_{\text{adsorbtion}} - T\Delta S_{\text{adsorbtion}}$$

To construct interaction schemes, charge (q_A, au), spatial (r, Å) characteristics and the amount of charge transfer (Δq, au) in model adsorption complexes were calculated.

Results. The Cr-pPAN cluster model obtained using the MM2 and PM7 methods is represented by a pPAN matrix with a chromium (III) oxide molecule embedded in the interplanar spacing (Fig. 1). The distance between interacting atoms inside the cavity was fixed at the level of 2.0–3.0 Å

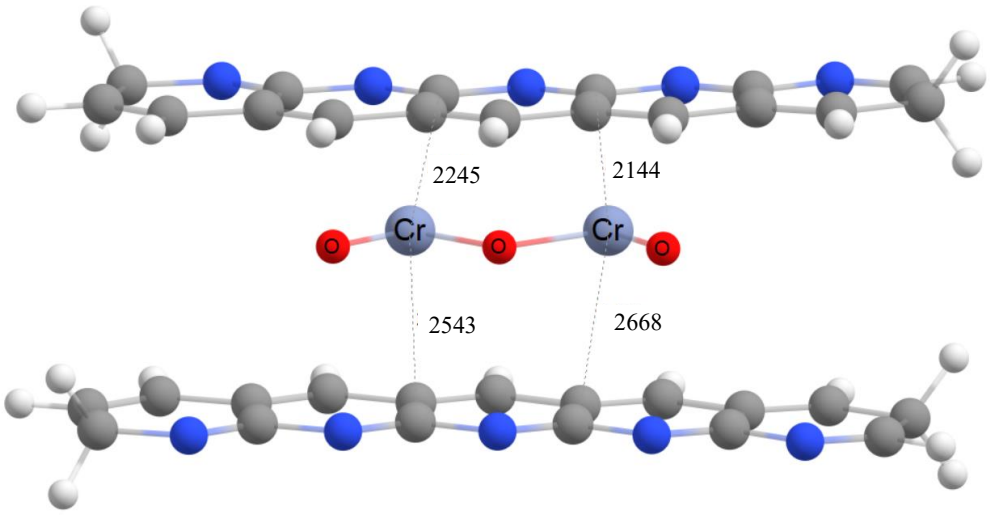

Fig. 1. A model of pPAN cluster modified by a chromium (III) oxide molecule

For example, below is a diagram of the hydrogen sulfide adsorption process:

$$Cr_2O_3(PAN)_2 + H_2S \Rightarrow [Cr_2O_3(PAN)_2 \ldots H_2S]$$

Similarly, adsorption schemes for other polluting gases were formed. Figure 2 shows a model using an example of the "Cr-pPAN – SO_2" adsorption complex.

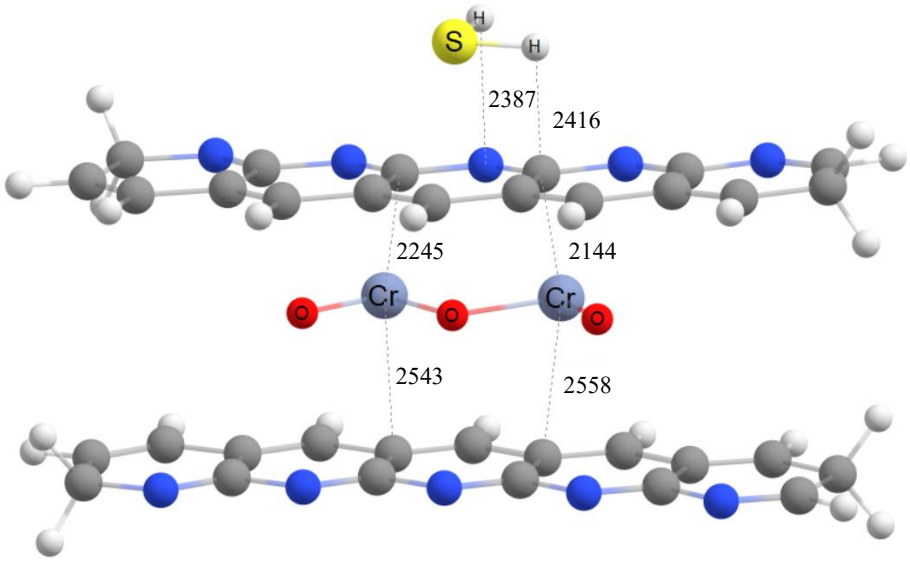

Fig. 2. Model of the "Cr-pPAN – SO_2" adsorption complex

Table 1 provides the calculated thermodynamic parameters of the processes of adsorption of polluting gases on the modified surface, in comparison with the data on the adsorption of these gases on the unmodified pPAN surface.

Table 1

Thermodynamic parameters of the processes of adsorption of polluting gases

Interaction model	Parameters at 298 K		
	ΔH, J/mol	ΔS, J/(mol·K)	ΔG, J/mol
H_2S…pPAN…Cr_2O_3..pPAN	–29.947	–413.888	93.392
NH_3…pPAN…Cr_2O_3..pPAN	–18.258	–295.817	69.896
CH_4…pPAN…Cr_2O_3…pPAN	–15.134	–264.146	63.581
CO_2…pPAN…Cr_2O_3..pPAN	–8.317	–232.773	61.050
NO_2…pPAN…Cr_2O_3..pPAN	–7.354	–232.601	61.961
SO_2…pPAN…Cr_2O_3..pPAN	–2.291	–208.585	59.868
O_3…pPAN…Cr_2O_3..pPAN	–17.887	–222.424	48.395
CO…pPAN…Cr_2O_3..pPAN	–41.647	–412.237	81.200
Cl_2…pPAN…Cr_2O_3..pPAN	–17.176	–217.306	47.580
H_2S…pPAN…pPAN	–1.215	–146.581	42.466
NH_3…pPAN…pPAN	–4.416	–160.438	43.394
CH_4…pPAN…pPAN	–3.197	–161.675	44.982
CO_2…pPAN…pPAN	–2.472	–150.947	42.510
NO_2…pPAN…pPAN	–0.759	–176.267	51.768
SO_2…pPAN…pPAN	–2.393	–181.495	51.693
O_3…pPAN..pPAN	–2.914	–280.125	80.563
CO…pPAN…pPAN	–2.192	–160.186	45.543
Cl_2…pPAN…pPAN	0.341	–153.047	45.949

In the adsorption complex "Cr-pPAN –pollutant gas", the internuclear distance from the extreme atom of the molecule of the studied pollutant gas to the nearest atom on the modified and unmodified pPAN surface was fixed at a level of more than 2.5 Å. These results are in good agreement with those obtained earlier [17] and confirm the presence of Van der Waals interaction occurring in the adsorption complex.

The charge change and electron density redistribution were not observed during the adsorption of pollutant gases on the unmodified pPAN surface (ΔH at the level of –3.0 kJ/mol).

It was established that the adsorption of SO_2 and NO_2 was equally possible both on the modified pPAN surface and on the unmodified pPAN surface, since as a result of the adsorption of these gases, there were no significant changes in the electron density on the surface of Cr-pPAN.

From the presented list of polluting gases, only CO gas shows off-scale results for the modified surface. In the process of adsorption, not only the maximum convergence between interacting atoms was carried out, but also an increase in the charge transfer index (Δq) from 0.3 au for an unmodified surface to 1.2 au for a modified surface.

Discussion and Conclusion. The calculated thermodynamic parameters of the system for standard environmental conditions, presented in Table 1, show that the adsorption of gases cannot be attributed to a spontaneous and self-existing process ($\Delta G > 0$). The general orderliness of the system established during the study of the adsorption processes of polluting gases demonstrates that adsorption is effective at high temperatures.

An increase in the charge in Cr-pPAN and a redistribution of electron density are most effective in the adsorption of polluting gases saturated with hydrogen atoms, namely, H_2S, NH_3, CH_4.

The occurrence of Van der Waals interaction between gases and the surface of Cr-pPAN has been confirmed during the adsorption of polluting gases on the surface of Cr-pPAN. This is justified by the absence of changes in the electron density at the Cr-pPAN polarity during interaction with polluting gases, as well as by the internuclear distance from the extreme atom of the molecule of the studied contaminant gas to the nearest atom of the modified and unmodified pPAN surface exceeding 2.5 Å.

In addition, the study showed that the introduction of chromium (III) oxide into the pPAN matrix contributed to an increase in the charge on nitrogen atoms (before/after: –0.366 au charge / –0.383 au charge). This led to a redistribution of electron density on carbon atoms in cycles (in the ortho position before/after: 0.357/0.428 au charge; in the meta position before/after: –0.159/–0.232 au charge).

Due to the fact that when chromium (III) oxide is introduced into the pPAN matrix, the charge on nitrogen atoms increases, it can be concluded that the chromium (III) oxide molecule has a positive effect on the semiconductor properties of pPAN.

Based on the calculations performed, it is confirmed that the adsorption of polluting gases (SO_2 and NO_2) is most likely on the surfaces of pPAN and Cr-pPAN.

Thus, the theoretical studies carried out allow us to conclude that the modification of pPAN with chromium (III) oxide molecules makes it possible to obtain a promising electrically conductive material with the property of selective adsorption of polluting gases, which can subsequently be successfully used in gas electronics.

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