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МОЛЕКУЛЯРНОЕ МОДЕЛИРОВАНИЕ АДСОРБЦИИ ГАЗОВ-ПОЛЛЮТАНТОВ НА КАДМИЙСОДЕРЖАЩЕМ ПОЛИАКРИЛОНИТРИЛЕ

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В публикации представлены теоретические исследования адсорбции газов-поллютантов на поверхности кадмийсодержащего полиакрилонитрила (Cd-полиакрилонитрила) при отсутствии и наличии в окружающей среде молекул воды и молекул кислорода. Определен перечень газов, к которым поверхность Cd-полиакрилонитрила может проявлять наибольшую чувствительностью. В качестве газов-загрязнителей выбраны диоксид азота, метан, аммиак, оксид серы (II), сероводород, озон, монооксид углерода, оксид углерода (II), хлор. Для моделирования в работе использованы программные пакеты: HyperChem, Gaussian 09, Chemoffice 2010. По итогам работы в HyperChem, Gaussian 09 получены модели макромолекул полиакринонитрила, из которых для получения кластера Cd-полиакрилонитрила выбрана макромолекула пентамера. Затем, реализуя метод молекулярной механики в Chemoffice 2010, а именно в подпрограмме Chem3D, произведено построение модели кластера Cd-полиакрилонитрила. Далее методом молекулярного моделирования определены термодинамические показатели систем: «кластер Cd-полиакрилонитрила – молекула газа», «кластер Cd-полиакрилонитрила – молекула кислорода», «кластер Cd-полиакрилонитрила – молекула воды», «кластер Cd-полиакрилонитрила – молекула кислорода – молекула газа», «кластер Cd-полиакрилонитрила – молекула воды – молекула газа». В результате молекулярного моделирования установлено, что Cd-полиакрилонитрил в атмосферном воздухе проявляет чувствительность к газообразному хлору и монооксиду углерода; в бескислородной среде – также к сероводороду. Результаты молекулярного моделирования подтверждают ранее полученные экспериментальные данные по оценке газочувствительности Cd-полиакрилонитрила и указывают на действие сил Ван-дер-Ваальса между поверхностью Cd-полиакрилонитрила и адсорбирующейся молекулой газа. Наличие или отсутствие в атмосферном воздухе молекул воды не должно сказываться на изменении чувствительности Cd-полиакрилонитрила к газам-поллютантам.

Ключевые слова: полиакрилонитрил, кадмий-содержащий полиакрилонитрил, молекулярное моделирование, влияние молекул воды (кислорода), адсорбция газов-поллютантов, силы Ван-дер-Ваальса

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MOLECULAR MODELING OF ADSORPTION OF POLLUTANT GASES ON CADMIUM-CONTAINING POLYACRYLONITRILE

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The paper presents theoretical studies of the adsorption of pollutant gases on the surface of cadmium-containing polyacrylonitrile (Cd-polyacrylonitrile) in the absence and presence of water molecules and oxygen molecules in the environment. The list of gases to which the Cd-polyacrylonitrile surface may have the highest sensitivity is determined. Nitrogen dioxide, methane, ammonia, sulfur oxide (II), hydrogen sulfide, ozone, carbon monoxide, carbon oxide (II), chlorine were chosen as pollutant gases. The following software packages are used for modeling: HyperChem, Gaussian 09, Chemoffice 2010. Polyacrylonitrile macromolecule models were obtained from HyperChem, Gaussian 09, from which a pentamer macromolecule was chosen to produce a Cd-polyacrylonitrile cluster. Then, implementing the molecular mechanics method in Chemoffice 2010, namely in the Chem3D subroutine, the Cd-polyacrylonitrile cluster model is constructed. Further, using the molecular modeling method, the following thermodynamic parameters were determined: «Cd-polyacrylonitrile cluster – gas molecule», «Cd-polyacrylonitrile cluster – oxygen molecule», «Cd-polyacrylonitrile cluster – water molecule», «Cd-polyacrylonitrile cluster – oxygen molecule gas molecule», «Cd-polyacrylonitrile cluster – water molecule – gas molecule». As a result of molecular modeling, it was established that Cd-polyacrylonitrile in the atmospheric air exhibits selective sensitivity to gaseous chlorine and carbon monoxide; in an oxygen-free environment – also to hydrogen sulfide. The results of molecular modeling confirm the previously obtained experimental data on the evaluation of the gas sensitivity of Cd-polyacrylonitrile and indicate the presence of van der Waals forces between the Cd-polyacrylonitrile and the adsorbed gas molecule. The presence or absence of water molecules in atmospheric air should not affect the change in the sensitivity of Cd-polyacrylonitrile to pollutant gases.

Key words: polyacrylonitrile, cadmium-containing polyacrylonitrile, molecular modeling, water (oxygen) molecules effect, pollutant gases adsorption, Van der Waals forces

INTRODUCTION

Modified polyacrylonitrile (PAN) is used to create supercapacitors, flexible electronic devices, self-cleaning coatings, photocatalysts, gas sensors, as a material for creating highly porous activated carbons [1-6]. The introduction of alloying additives into the PAN allows one to change its physicochemical, electrical, mechanical properties, which makes it possible to synthesize composite materials with given parameters of properties. After thermal treatment by IR annealing, PAN acquires the properties of sensitivity to atmospheric air gases at room temperature [7-12] and can serve as the basis for the synthesis of metal-containing composites, which, in turn, have the property of selective sensitivity to polluting gases. To improve the metrological indicators of polyacrylonitrile films, they often resort to varying the time and temperature parameters for producing PAN films, as well as the type and concentration of modifying additives (transition metal salts) [9, 10]. One example of a PAN-based nanocomposite material is Cd-PAN, which has selective sensitivity to hydrogen sulfide [10, 11]. However, to obtain a highly efficient gas-sensitive material, theoretical studies of the causes of the selective gas-sensitivity of Cd-PAN films are required, as well as the effect of various components in the analyzed air-gas medium on the adsorption of gases.

The purpose of this paper is to study the gas sensitivity of Cd-PAN according to the results of molecular modeling of the interaction of a Cd-PAN cluster with molecules of pollutant gases with different atmospheric air composition.

RESEARCH TECHNIQUES

The method of quantum chemical calculations in the HyperChem program using semi-empirical computational schemes (MNDO) was used to obtain spatial configurations of PAN pentamer macromolecules. Further, for maximum accuracy of the results in the Gaussian09 software package using the Pople base set (6-31 G*) within the framework of the density functional theory (DFT), we calculated the thermodynamic indicators of PAN macromolecules [13-15].

To obtain the Cd-PAN cluster and estimate its gas sensitivity, the molecular modeling method (or minimization of the potential energy of the system in a modified version of the force field (MM2) developed by Ellinger [16]) was used in the Chem3D sub-program of the Chemoffice program [13, 17-21].

Synthesis of Cd-PAN films is carried out by the method of pyrolysis under the influence of IR radiation under low vacuum [10]. Cadmium (II) chloride dissolved in dimethylformamide is used as the alloying component. As a rule, IR annealing of Cd-PAN films is carried out at temperatures not exceeding 350-400 °C. Since the melting point of cadmium chloride is 568.5 °C [22], cadmium salts are likely to be present in films of thermally stabilized Cd-PAN).

According to the foregoing, as a model of a Cd-PAN cluster, we take a system consisting of chains of macromolecules of PAN and cadmium chloride molecules located in the interlayer space. To simplify, we consider a system of 2 parallel oriented macromolecular chains of pentamers and one molecule of cadmium parallel to each other. When implementing the molecular mechanics method in the Chem3D software package, we set different positions for the location of the cadmium chloride molecule: (1) from the edge and (2) in the center of the interlayer space (Fig. 1). We establish that the most energetically favorable arrangement of $CdCl_2$ is in the central part of the interlayer space (2).

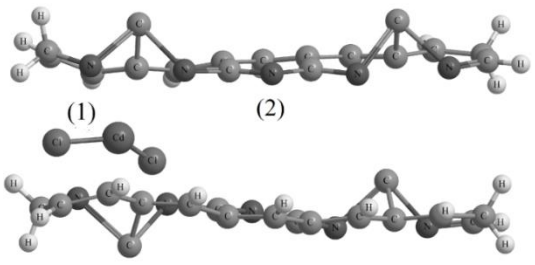


Fig. 1. Introduction of cadmium chloride in the PAN system: (1) – on the edge of the PAN cluster (E_{min} = 1467.42 kJ / mol); (2) – in the center of the PAN cluster (E_{min} = 1401.22 kJ / mol)
Рис. 1. Внедрение хлорида кадмия в систему ПАН: (1) – с краю кластера ПАН (E_{min} = 1467,42 кДж/моль); (2) – в центр кластера ПАН (E_{min} =1401,22 кДж/моль)

At the next stage, the possibility of adsorption of pollutant gases (nitrogen oxide (IV), ammonia, sulfur oxide (II), hydrogen sulfide, ozone, carbon oxide (IV), carbon oxide (II), chlorine) on the surface of the Cd-PAN cluster was investigated. At the same time, different positions of gas molecules were set: (1) – inside the cluster and (2) – (12) – in the middle of the cluster at a distance of 2-10 Å from the surface (Fig. 2).

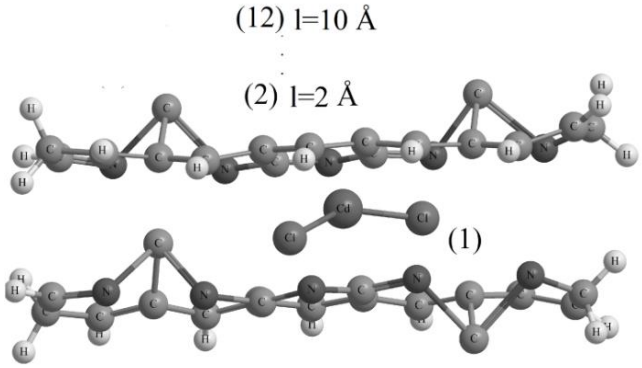


Fig. 2. The location of gas molecules at interacting with the surface of a Cd-PAN cluster
Рис. 2. Расположение молекул газов при взаимодействии с поверхностью кластера Cd-ПАН

At this stage, the thermodynamic characteristics (steric energy of the system (E_{min}), binding energy (ΔE), energy minimum points (l_{min})) and geometric indicators (distances between gas molecules and the Cd-PAN cluster (l)) were identified.

Then, similarly to the above, the systems "PAN cluster - oxygen molecule" and «PAN cluster – water molecule» were studied, namely the steric energy of this system ($E_{Cd\text{-}PAN + O_2}$ and $E_{Cd\text{-}PAN + H_2O}$), the binding energy between the oxygen / water molecule and the surface of the PAN cluster (ΔE), the points with the minimum energy (l_{min}), and also the distances between the molecules of pollutant gases and the oxygen molecule (L_{O_2}) / water (L_{H_2O}). At the last stage of implementation of the molecular modeling method, the systems Cd-PAN cluster – oxygen molecule – gas molecule and Cd-PAN cluster – water molecule – gas molecule were investigated.

According to the results of the comparison of the thermodynamic parameters of the studied systems, first of all their steric energies, the possibility of interaction of gas molecules with Cd-PAN was evaluated.

RESULTS AND DISCUSSION

As a result of molecular modeling of the Cd-PAN cluster, it was found that the steric energy of this cluster is 1401.22 kJ/mol, the steric energy of

the «Cd-PAN cluster – oxygen molecule» system is 1397.62 kJ/mol, and the steric energy of the «cluster Cd-PAN is a water molecule» – 5206.33 kJ/mol. Based on the obtained results, it can be concluded that oxygen adsorption is most likely due to the fact that E_{min} Cd-PAN + O_2 < E_{min} Cd-PAN. In this case the interaction with the water molecule of this cluster is excluded (E_{min} Cd-PAN << E_{min} Cd-PAN+H_2O), therefore, the effect of humidity on the adsorption of pollutant gases in this case is unlikely. This is also confirmed by the study [11]. The results of molecular modeling of the adsorption of pollutant gases on the surface of Cd-PAN in various gaseous medium are presented below in tables 1-3 and in fig. 3 and 4.

Table 1

Steric energy of the system Cd-PAN cluster – water / oxygen molecule – gas molecule

Таблица 1. **Стерическая энергия системы «кластер Cd-ПАН – молекула воды / кислорода – молекула газа»**

Gas	E_{min}, kJ/mol		
	Cd-PAN	Cd-PAN + H_2O	Cd-PAN + O_2
Cl_2	1358.48	5206.33	1392.97
CO	1398.45	5175.07	1389.57
O_3	6271.05	7383.83	2446.88
NO_2	3545.87	7782.97	10156.85
H_2S	1395.90	5485.63	1706.88
CO_2	2061.65	5665.42	2081.17
SO_2	2288.75	6042.02	2278.06
NH_3	4787.03	7263.41	4864.13

Table 2

Bond energy of the system Cd-PAN cluster – water / oxygen molecule – gas molecule

Таблица 2. **Энергия связи системы «кластер Cd-ПАН – молекула воды / кислорода – молекула газа»**

Gas	ΔE, kJ/mol		
	Cd-PAN	Cd-PAN + H_2O	Cd-PAN + O_2
Cl_2	12.46	9.09	0.71
CO	2.85	4.44	4.15
O_3	18.98	8.34	1.76
NO_2	86.10	6.45	4.78
H_2S	5.36	8.25	1.38
CO_2	8.88	46.84	4.73
SO_2	3.18	22.12	6.33
NH_3	9.43	12.99	1.68

The minimum values of steric energy were obtained for the interactions of the Cd-PAN cluster with chlorine and carbon monoxide molecules and hydrogen sulfide. Regardless of whether there are oxygen or water molecules in the environment, Cd-PAN films will be sensitive to Cl_2 and CO. When interacting in an oxygenated and humid environment of Cd-PAN with H_2S molecules, the energy costs will be relatively low due to the small ΔE_{min} value, which may indicate the presence of hydrogen sulfide sensitivity under the indicated conditions.

Table 3

Points with the minimum energy of the Cd-PAN cluster – water / oxygen molecule – gas molecule" system and the distance of gas molecules from H_2O/O_2

Таблица 3. **Точки с минимальной энергией системы «кластер Cd-ПАН – молекула воды / кислорода – молекула газа» и расстояния молекул газов от H_2O/O_2**

Gas	l_{min}, Å			L,Å	L,Å
	Cd-PAN	Cd-PAN+H_2O	Cd-PAN+O_2	H_2O	O_2
Cl_2	3.5	3.5	6	5.4	3.2
CO	3.7	3.2	3	2.9	2.7
O_3	3.7	6	6	2.7	3.5
NO_2	2.5	3.7	6	2.7	5.8
H_2S	3.7	3.5	6	3.1	4.7
CO_2	3.2	3.4	3	3.3	3.1
SO_2	4	3.2	3	2.6	3.4
NH_3	3	2.5	4	4.7	2.7

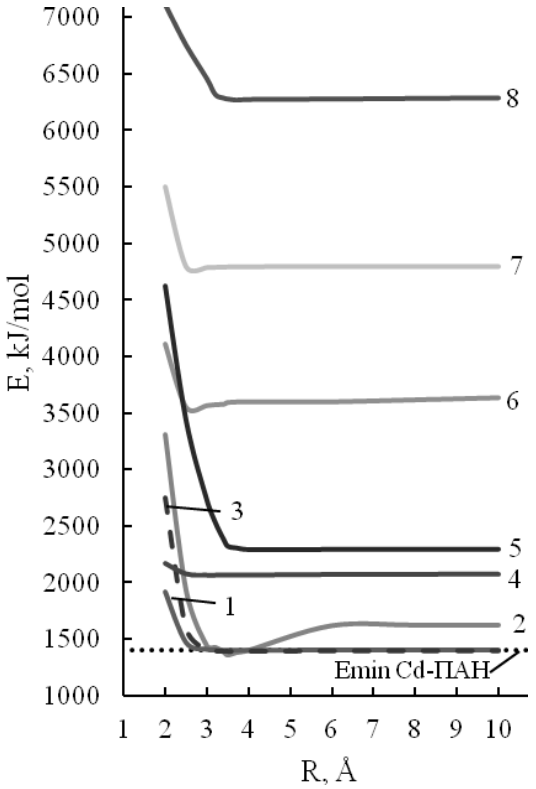


Fig. 3. The dependence of steric energy on the distance to the gas molecule for the system «cluster Cd-PAN – gas molecule». 1 – CO; 2 – Cl_2; 3 – H_2S; 4 – CO_2; 5 – SO_2; 6 – NO_2; 7 – NH_3; 8 – O_3

Рис. 3. Зависимость стерической энергии от расстояния до молекулы газа для системы «кластер Cd-ПАН – молекула газа». 1 – CO; 2 – Cl_2; 3 – H_2S; 4 – CO_2; 5 – SO_2; 6 – NO_2; 7 – NH_3; 8 – O_3

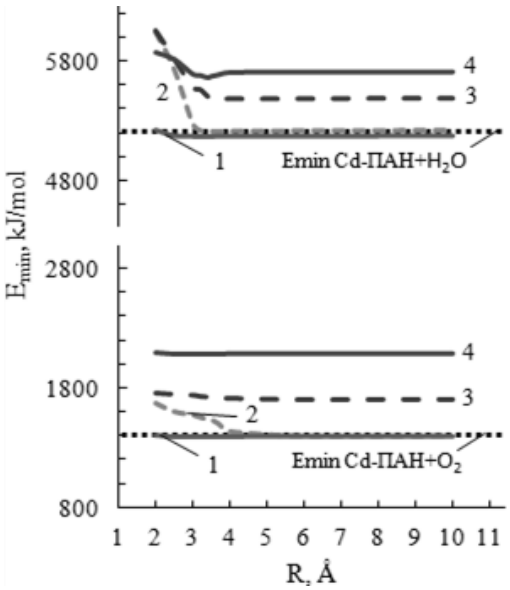
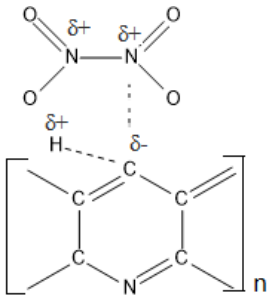


Fig. 4. The dependence of steric energy on the distance to the gas molecule for the systems «cluster Cd-PAN – oxygen molecule – gas molecule» (at the top) and «Cd-PAN cluster – water molecule – gas molecule» (at the bottom): 1 – CO; 2 – Cl_2; 3 – H_2S; 4 – CO_2

Рис. 4. Зависимость стерической энергии от расстояния для систем «кластер Cd-ПАН – молекула кислорода – молекула газа» (вверху) и «кластер Cd-ПАН – молекула воды – молекула газа» (внизу): 1 – CO; 2 – Cl_2; 3 – H_2S; 4 – CO_2

The analysis of the obtained binding energies (ΔE) between the gas molecules and the cluster surface showed that in most cases, van der Waals interaction forces arise between the components of the system. An exception is the interaction of nitrogen dioxide molecules with a Cd-PAN cluster in an oxygen-free environment, where the binding energy reaches a higher value than in the case of other gases, which is explained by the possible coordination interaction of PAN with NO_2 dimers according to the following scheme:



Since in the case of adsorbed nitrogen dioxide molecules, sufficiently high energy costs are required, exceeding the energy of the Cd-PAN cluster (Cd-PAN / Cd-PAN + O_2), the interaction of NO_2 with the cluster surface at standard temperature is excluded.

For the gases considered, the smallest points with the minimum energy are in most cases within 2.5-3.7 Å from the Cd-PAN cluster (Table 3). This distance between the gas molecule and the surface of the cluster allows intermolecular interactions, but excludes the possibility of overlapping electron clouds and the appearance of a chemical bond. For this reason, the appearance of a chemical bond is also excluded between the oxygen / water molecule and the gas molecule (L_{O_2}, L_{H_2O}).

CONCLUSION

Studies carried out by molecular modeling have established that Cd-PAN will be sensitive to chlorine, carbon monoxide and, in an oxygen-free environment, also to hydrogen sulfide in atmospheric air. Assuming that the binding energy in most cases does not exceed the value of 20 kJ/mol, we can assume that Van der Waals forces act between the gas molecules and the Cd-PAN surface.

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