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**THE ORGANIC COMPOUNDS AS INHIBITORS OF FUNGAL CORROSION OF STEEL: QUANTUM CHEMICAL MODELING OF INHIBITOR PROTECTION**

**ОРГАНИЧЕСКИЕ СОЕДИНЕНИЯ КАК ИНГИБИТОРЫ МИКОЛОГИЧЕСКОЙ КОРРОЗИИ СТАЛИ: КВАНТОВОХИМИЧЕСКОЕ МОДЕЛИРОВАНИЕ ИНГИБИТОРНОЙ ЗАЩИТЫ**

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*Abstract.* In a published scientific article presents modeled using quantum chemistry package HyperChem version 8.0.7 using semiempirical method ZINDO/1 the process of adsorption of organic sulfur-containing compounds such as iron (available in steel St3S (Poland) in the amount of 97%). Compare and explain the protective effects of corrosion depending on the extent of cathodic polarization of the metal model specimen.

This way with high accuracy reflects the process of corrosion protection with mycological content (*Penicillium chrysogenum* cells) by the chemisorption of organic compounds on the metal surface with the formation of complex compounds. Inhibitor protection carried out with a sample of the metal cadmium plating protected with a current density of 4 A/dm<sup>2</sup>. As a comparison, the properties and characteristics of some complexes responsible for metal protection, will be referred to secondary data obtained from protected metal cadmium plating sample 1–3a/dm<sup>2</sup>. In the research process were obtained and analyzed: the charges on the heteroatoms, the charge density (1 atom of iron), the composition of the resulting compounds Fe<sub>a</sub>←[SMY], as well as energy diagrams in the formation of the adsorption complex of the studied molecules.

Absolute linear graph type “Z% — Feρ<sub>q</sub>”, so the charge density on the iron is a powerful predictive parameter in the mission of inhibitor (at various concentrations) to protect steel from corrosion, without the use of a screening method. Knowledge of the partial effective charges of helping to determine the most powerful adsorption centers belonging to a specific molecule inhibitor. Changing values frontier orbitals helps to assess the stability of the adsorption complex inhibitor compounds with metal atoms.

*Аннотация.* В работе представлен смоделированный при помощи квантовохимического пакета HyperChem версии 8.0.7 при помощи полуэмпирического метода ZINDO/1 процесс адсорбции органических серосодержащих соединений на железе (имеющемся в стали Ст3 (точнее марка St3S, Польша) в количестве 97%). В рамках статьи представлено сравнение и объяснение защитных эффектов от коррозии в зависимости от степени катодной поляризации испытуемого образца металла.

Ингибиторная защита осуществляется в отношении образца, покрытого металлическим кадмием, защищенного катодной плотностью тока 4 А/дм<sup>2</sup>. В качестве сравнения, будут отражены «вторичные» данные по защите образца, покрытого металлическим кадмием, защищенного катодной плотностью тока 1...3 А/дм<sup>2</sup>.

Такой подход, как будет показано далее, с высокой точностью отражает процесс защиты от коррозии с микологическим контентом (клетки *Penicillium chrysogenum* Thom (1910)) путем хемосорбции органического соединения на поверхности металла с образованием комплексного соединения. В процессе исследования были получены и проанализированы: заряды на гетероатомах, плотность заряда (на 1 атом железа), состав получившихся соединений  $Fe_x$  [ИМ Y], а также энергетические диаграммы при образовании адсорбционного комплекса из исследуемой молекулы.

*Keywords:* HyperChem, corrosion, *Penicillium chrysogenum*, adsorption, St3S steel, the partial effective charges.

*Ключевые слова:* HyperChem, скорость коррозии, грибы *Penicillium chrysogenum*, адсорбция, сталь Ст3, парциальные эффективные заряды.

### *Background*

Biological damage of the material is any undesirable change in the properties caused by the vital activity of organisms. Biological corrosion of metals is a part of the problem of biological damage. The most active agents of damage are micro — filamentous fungi and bacteria, which accounted for 20% of total damage. Many bacteria and filamentous fungi form in the metabolism of ammonia, hydrogen sulfide, and various organic acids, most of which are characterized by high corrosion activity. In the process of development of microorganisms, being acceptors on metal surfaces, destroy inhibitors that protect the metal, and stimulate its corrosion. Biological corrosion of metal products, structures usually occur in moist conditions when dirty. The most active agents of bio-corrosion of metals and coatings are fungi [1].

The most promising for the fight against metal corrosion in the presence of filamentous fungi the use of organic inhibitors possessing besides biocidal activity. But because of the addiction of lower organisms to biocides used for a long time, they need to be updated periodically. Therefore, a search of new organic compounds, electrochemical corrosion inhibitors possessing biocidal activity at lower organisms.

Not too many microbiological corrosion studies conducted [2, 3]. Many studies have been conducted in the Tambov State University and Baltic Federal University (Russia). Corrosion of different metals in aggressive acidic, for example, [4–6] and salt [11] medium are investigated a very large number of scientists worldwide.

Many of the organic compounds that perform the mission of protecting corrosion [4, 6, 10], have been investigated by the approach “structure-property” using the Pearson correlation coefficient, for example, [4, 2, 12, 13]. Simulation according reactivity of organic compounds was undertaken in the past [14], in particular, the simulation of adsorption on the metal clusters of organic compounds described hypothetical cluster where the metal surface [15, 16]. Contributed by the author changes in cluster modeling method suggest it is an organic compound adsorption capabilities with regard, in particular, to iron, and therefore there is a new value of the “charge density on the iron”, i. e. the proportion of the electron density, which passed from the organic compound converted for an individual iron atom [17].

### *Methods*

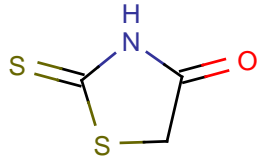
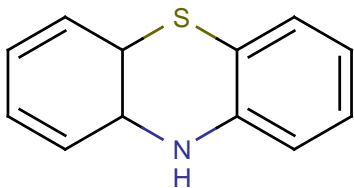
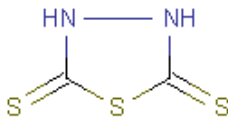
*A variety of microbiological corrosion system.*

In the article investigated the heterogeneous thermodynamic system of closed type “St3S+Cd/nutrient medium of Chapek + *Penicillium chrysogenum* cells”. Samples of steel were parameters 20×50×1 mm, and were covered from cadmium sulphate electrolyte of cadmium plating with a current cathodic density of 4 A / dm<sup>2</sup>. Then, with cadmium plated steel samples were made in the inoculated nutrient medium of Chapek with *Penicillium chrysogenum* cells.

Using organic inhibitors and their method of application in the corrosion system  
 Study was subjected to the following sulphur-containing compounds (see Table 1).

Table 1.

USEFUL AS INHIBITORS OF ORGANIC COMPOUND

Abbreviation of inhibitor	Name	Structural formula	Molecular weight
SM 1	4-oxo-2-thiooxo-1,3-thiazolidin		133.18
SM 2	10H-dibenzo-[b,e]-1,4-thiazin		199.27
SM 3	1,3,4-thiadiazolidine-2,5-dition		149.91

It's were introduced into the cadmium plating electrolyte concentrations 1, 2, 5 mmol / l. After the passage of the current SM spontaneously built into the electrodeposited cadmium. Such a process was invented earlier [3], and was tested for the first time at the Department of Chemistry of the Baltic Federal University.

*The protective effect against corrosion*

Data on corrosion rates obtained with gravimetric analysis, and that were described below. These values are as follows

Table 2.

PROTECTIVE EFFECTS OF CORROSION AT A CURRENT DENSITY OF 4 A / DM<sup>2</sup> WITH THESE SUBSTANCES

SMY	Concentration of corrosion inhibitors in the microbial system		
	1 mmol / L	2 mmol / L	5 mmol / L
	The protective effect against corrosion, %		
SM 1	74	78	79
SM 2	83	84	84
SM 3	79	79	80
Control	<u>77</u>		

*Technology of experiment*

In this work, the data are indicated (see Table 2), which occur when cadmium plating steel sample (it is a cathode) at a cathodic current density of 4 A/dm<sup>2</sup> inhibitors (Table 1) at 1, 2, 5 mmol / l. The author will also data that appear when cadmium plating of steel samples at the cathode 1 ... 3 A/dm<sup>2</sup> current density. But these data will lead only to test the hypothesis put forward by the

author, explaining that the protective effect of corrosion to a large extent will depend on the stability of iron complexes. For the main aspects of the author of the selected value, corresponding to an arbitrary value of the current density of 4 A/dm<sup>2</sup>.

*The technology of quantum chemical calculations*

The calculation was performed with HyperChem 8.0.7. Software, empirically, the limit was set by the number of iron atoms: a number *a*, when out of (*a* + *b*) given iron atoms carrying zero charge number *b*. Then it was assumed that the SM donor possibilities exhausted. Equation electrophilic  $a\text{Fe} + \text{SMY} = \text{Fe}_a\leftarrow[\text{SM Y}]$ , reaction where iron atoms - acceptors, which are charged negatively. Finding the values of quantum chemical descriptors held level theory OPLS / AM1 / ZINDO / 1. Mesomeric effect was taken into account, which is manifested in different parts of the investigated SM. In the following controlled descriptors of electronic structure: charges on heteroatoms (by Mulliken), the energy of frontier orbitals (HOMO, LUMO [18], 1LUMO [19] in the formation of the adsorption complex of SM  $\text{Fe}_a\leftarrow[\text{SMY}]$ ), the resulting composition  $\text{Fe}_a\leftarrow[\text{SM Y}]$ , where the SM acts as a ligand. Based on these characteristics will be calculated from the data file .out: the charge density on the iron (1 atom of Fe), global and local electrophilicity, consider the complex structure. In the file-job was posted mesomeric effect on the structure of the ion.

*Results*

*The heteroatoms as the adsorption sites*

The generated results are summarized in Table 3.

Table 3.

VALUES OF THE CALCULATED QUANTUM CHEMICAL DESCRIPTORS OF THE INVESTIGATED HETEROCYCLES AND COMPLEX COMPOUNDS ON THEIR BASIS

<i>Codes of substances Y format</i>	<i>SM 1</i>	<i>SM 2</i>	<i>SM 3</i>
$\omega$	0.163	0.031	0.171
$\omega_S$	0.079	0.016	0.077
$\omega_N$	0.031	0.005	0.045
Effective charges on heteroatoms	${}_tq_S = -0.167$	${}_tq_S = -0.270$	${}_tq_S = -0.123$
	$q_N = -0.229$	$q_N = -0.236$	$\Sigma q_N = -0.214$ ( ${}_1q_N = -0.107$ )
The composition of the substance complexes	$\text{Fe}_9\leftarrow[\text{SM 1}]$	$\text{Fe}_{14}\leftarrow[\text{SM 2}]$	$\text{Fe}_8\leftarrow[\text{SM 3}]$
$\omega$	3.989	2.032	2.134
Effective charges on heteroatoms	${}_tq_S = 0.318$	${}_tq_S = 0.259$	${}_tq_S = 0.329$
	$q_N = -0.038$	$q_N = -0.079$	$\Sigma q_N = -0.081$ ( ${}_1q_N = -0.050$ ) ( ${}_2q_N = -0.031$ )
$\text{Fe}\rho_q$	-0.264	-0.367	-0.299

*The energies of the frontier orbitals*

Energy diagram for the  $a\text{Fe} + \text{SM Y} = \text{Fe}_a\leftarrow[\text{SM Y}]$  are presented in Figures 1–3:

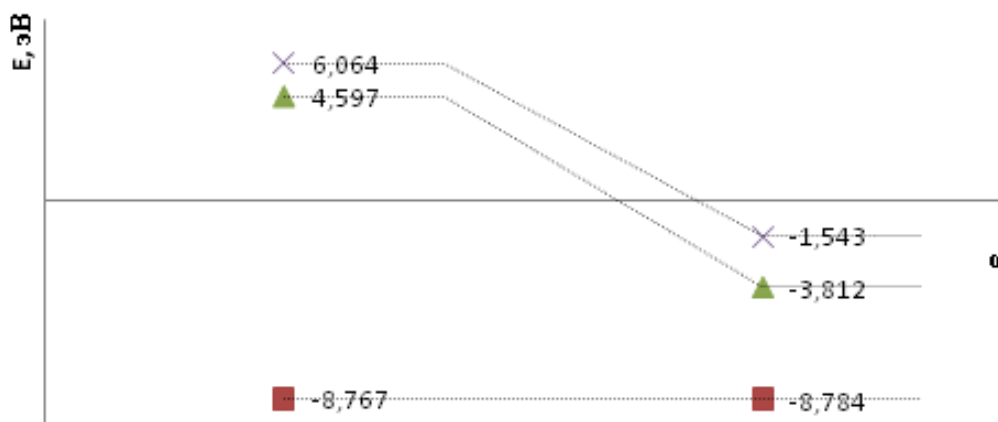


Figure 1. The change of position of energy levels of HOMO (■), LUMO (▲), 1LUMO (×) in the formation of the adsorption complex (right) with SM 1 (left).

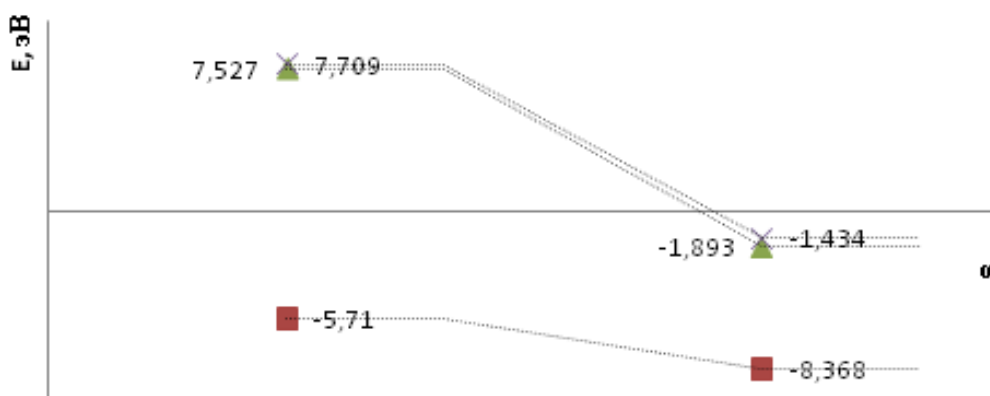


Figure 2. The change of position of energy levels of HOMO (■), LUMO (▲), 1LUMO (×) in the formation of the adsorption complex (right) with SM 2 (left).

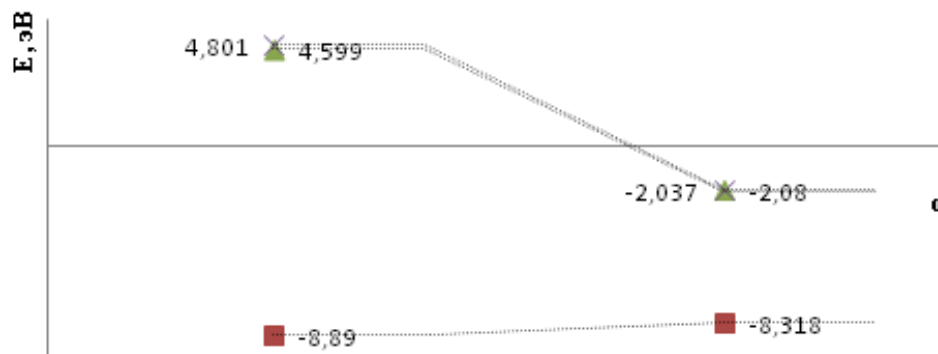


Figure 3. The change of position of energy levels of HOMO (■), LUMO (▲), 1LUMO (×) in the formation of the adsorption complex (right) with SM 3 (left).

### Discussion of results

#### Donor activity of heteroatoms

According to Table 1, the energy of LUMO of organic iron-containing complexes is correlated with the number of sulfur atoms: the energy is higher, the smaller the number of sulfur atoms, with worse electron density is drawn.

In this work tracked donor activity of nitrogen atoms and tiasulfur. This approach is the most objective, since such groups are typical for all 3 compounds.

According to table 1, it is obvious that teaser is a strong donor of electron density. The studied compounds can be a number of “SM2-SM 1-SM3”, i. e. the relationship as the size of the molecules (the highest donor properties), and the number of sulfur atoms (the more the molecule tiagroup, the donor properties worse).

Unlike tiasulfur atoms, the donor properties of the nitrogen atoms do not depend on the size of the molecule. So, the donor properties are the most of SM3, where the nitrogen atoms are present in the amount of two, but despite this, the total charge on SM of about the same as the rest of the molecules (from which it follows that the properties they are similar to the nitrogen atoms of the 2 other SM). Further they descend in the series “SM 1–SM2”. Apparently, a crucial role is played by the pair of nitrogen atom with the other structures. In the case of SM 1 pairing occurs as with tiasulfur and ketogroup, while in the case of the SM2 — only with the benzene rings.

#### The global electrophilicity and the stability of the adsorption iron complexes

Considering the magnitude of the global electrophilicity, it is obvious that such reduction is in the number of “SM3–SM 1-SM2”, which likely correlates with the number of sulfur atoms in the form of tiagroup. In a series of “SM3- SM 1” fall is not so sharp, since the role of the second atom tiosulfur assumes ketogroup, the disappearance of both fragments leads to an almost zero value of the global electrophilicity.

Obviously, the results on the global electrophilicity the most informative. Examining it, it is possible to assess the sustainability of ironcomplexes that this work will be done for the first time. To review available Figure 4

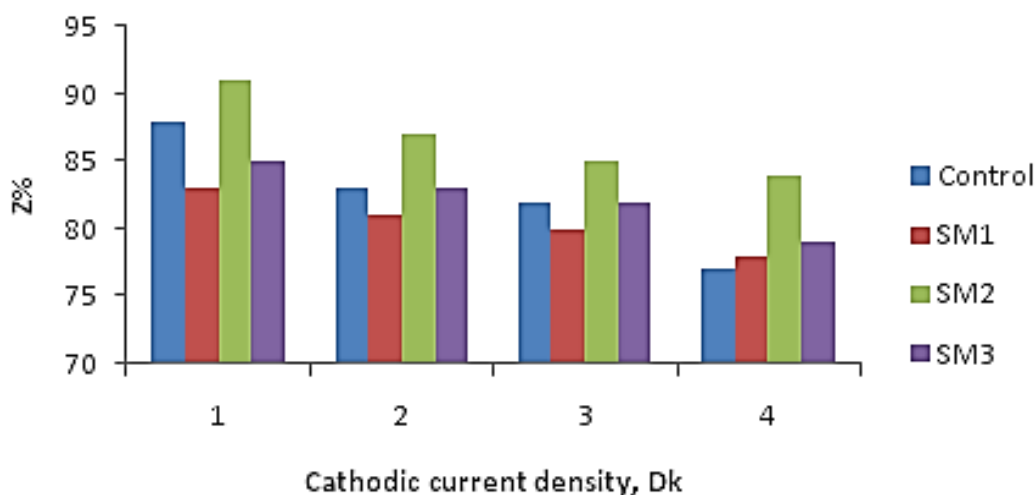


Figure 4. Effect of organic additives (concentration of 2 mmol / l) on the protective effect (%) depending on the current density in the presence with *Penicillium chrysogenum*.

Figure 4 shows that the decrease in Z% with growth  $D_k$  occurs abruptly, only the test series shows a very small decrease in a linear Z%. Comparing the magnitude of the protective effect of anticorrosive cathodic current density at 1, 2, and 3 A / dm<sup>2</sup>, there are larger quantities while maintaining the overall picture values corrosion protective effects. The visible and concrete (and



used almost) Z%, as described in Table 2, is generated by two factors (in addition to the biocide): 1) the ability to be adsorbed on the surface of the cathodic polarized metal organic inhibitor SM Y and 2) resistant  $Fe_a \leftarrow [SM Y]$ . Power manifestations of these factors depends on the value of  $D_k$ . When the author of the selected value  $D_k = 4 \text{ A / dm}^2$  (where the nucleophilic properties of the sample peak) it is best to adsorb the least electrophilic SM Y, i.e., SM 2. Here, in the most strongly established Fe-SM 2 chemisorption communication, providing effective shielding steel sample. The percentage of cadmium coatings (because it is thin layer) is not very high. Speed  $14Fe + SM 2 = Fe_{14} \leftarrow [SM 2]$  reaction will be as much as possible.

The stability of the complex at a cathode current density of  $4 \text{ A / dm}^2$  will be determined by susceptibility  $Fe_a \leftarrow [SM Y]$  to an excess of electron density that best transports  $Fe_{14} \leftarrow [SM 2]$  as well. Electrophilic  $Fe_9 \leftarrow [SM 1]$  is destroyed.

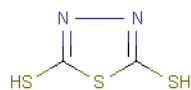
When the value of  $D_k < 4$  protective effect up to 90%, this is due to a smaller surplus of electron density on the steel cadmium plate. Electrophilic both  $Fe_9 \leftarrow [SM 1]$  and  $Fe_8 \leftarrow [SM 3]$  preserved better. Nucleophilic sample properties become weaker, so also is weaker will be the adsorption of SM 2, but more SM 1 and SM 3, so the most useful effect have connections built into electroplating Cd of sulphate electrolyte formed with a smaller cathode current density ( $1 \text{ A / dm}^2$ ) which is actually used in machine-building, shipbuilding, aircraft engine and electronic factories, cadmium plating numerous assortment of products [20].

#### *The local electrophilicity and donor abilities of heteroatoms*

There is high value of local electrophilicity. These values indicate strong tendency of donating electron density on iron. Extremely low values of the local electrophilicity of SM 2 show that the electron pair of the nitrogen atom and the sulphur atom are involved in conjugation with benzene rings. Equal to the value of the local sulphur electrophiles of SM 1 and SM 3 show that the electron pair of the nitrogen atom and the sulfur atom is equivalent to participate in donating electron density.

#### *Energy diagram for the reaction of appearance of iron complexes*

According to the Figures 1–3, it is obvious that the pattern of the orbitals of complexes and initial SM each other again, full overlay LUMO and 1LUMO is implemented in SM2 and SM3, which indicates the aromaticity of these compounds (2 is aromatic due to the presence of benzene



rings, 3 is in tautomeric equilibrium with [19], subject to the Hückel's rule; due to tautomerism the energy levels in Figure 3 below). Apparently, the presence of ketogroup in part 1 generates a strong separation energies LUMO and 1LUMO. The same factor obviously affects neumegen donor properties as complex and original to SM (since the energy of HOMO does not change).

#### *The density of the effective charge attributable to the iron atom*

The dependence of corrosion rate at concentration of inhibitor 1, 2, 5 mmol/L charge density on iron is in Figure 5:

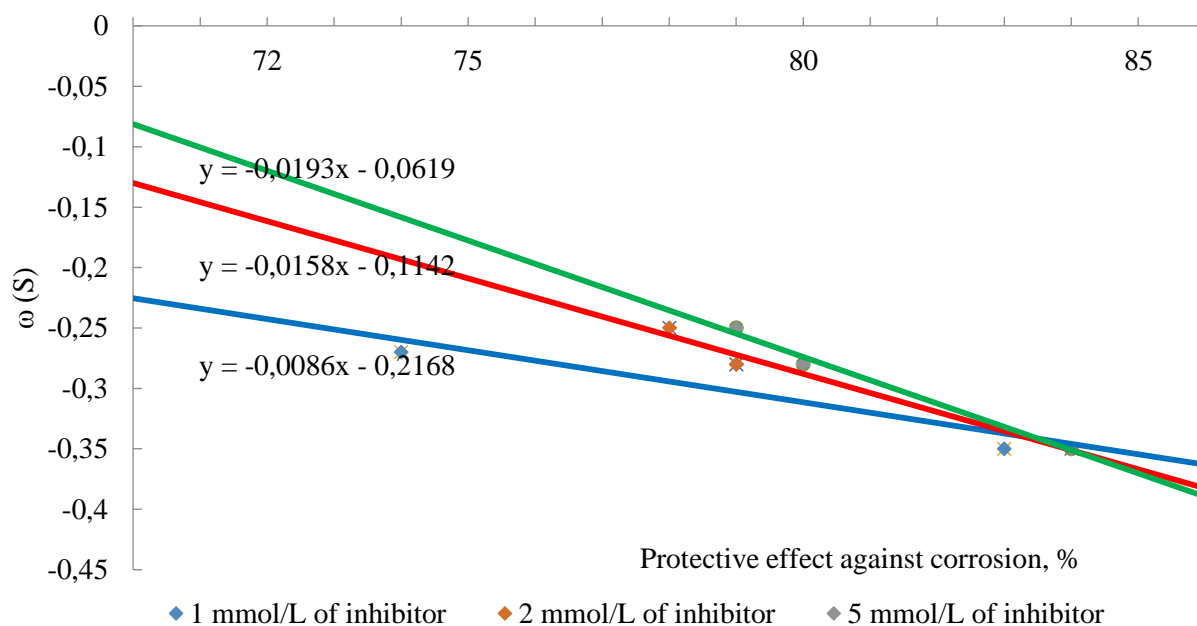


Figure 5. Characteristics of the importance of the charge density on the iron atom (cathodic current density is  $4 \text{ A / dm}^2$ ).

It is obvious that the inhibitory effect begins to occur when the value of the charge density on iron over  $\text{Fepq} = -0.15$ . It is also evident that at a concentration of  $5 \text{ mmol/L}$  this dependence is strongest, i.e. at the more dramatic increase in density has a sharper decrease in corrosion rate. At concentrations, less than high such dependence is preserved but is expressed less sharply.

When the value of the protective effect of  $84\%$  dependence itself from the charge density on iron is lost, the latter receives a steady value  $\text{Fepq} = -0.35$  [21].

### Conclusion

Application of article approach, such as lack of hydration molecules, the use of pure iron atoms cluster instead of steel, neglect of participation in the adsorption of molecular hydrogen sulphide and its ions, semi-empirical methods of calculation sand modeling obviously do not impose the print on the accuracy and predictive ability of the author improved cluster modeling theory. This enhancement allows you to get more information about protection of inhibitors of metal than the traditional and generally accepted theory. The improved method of quantum chemical modeling provides a much more comprehensive set of data that can serve as an effective tool for forecasting. Because ironcomplexes is not seen as superficial, and as an independent organic compound (or rather, the adduct) with well-defined chemical composition, is similar to  $\pi$ -complexes may be calculated as the actual value of the electronic tags last structure and function of Fukui. This represents a great promise, because currently the selection of microbial corrosion inhibitors increasingly performed quantum-chemical methods of prediction, not a screening method [22].

There is no doubt that a significant role in shaping improvements quantum chemical modeling belongs to the tremendous development of the power of new versions of quantum chemical programs, as well as the full development of visual imaging software. As soon as supercomputers are increasingly becoming an essential attribute of any area of the economy, all of the above approach will be less needed along with an increase in the level of quantum-chemical theory.

*Abbreviations:* SM — the studied molecule; eV — Off-system unit called the electron-volt;  $q_S$  — charge on the tiasulfur atom;  $q_N$  is the charge on the nitrogen atom;  $q$  is the charge on a



particular atom;  $2q$  is the charge on another atom specific;  $\Sigma q$  is a value of the total charge, is given by:  $\Sigma q = 1q + 2q$  HOMO the highest filled molecular orbital; LUMO — the lowest free molecular orbital;

1 LUMO — orbital, the next lowest free molecular orbital;  $\omega$  — the value of the global electrophilicity;  $\omega_s$  is the magnitude of the local electrophilicity particular atom;  $Fe\rho_q$  is the charge per one atom of iron (density of charge);  $D_k$  — cathodic polarization mode: cathodic current density;

#### Competing interests

The author declares that they have no competing interests.

#### References:

1. Iyer, R. N., Pickering, H. W., Takeuchi, I., & Zamanzadeh, H. (1990). Hydrogen Sulfide Effect on Hydrogen Entry into Iron. A Mechanistic Study. *Corrosion*, 46, (6). 460–467.
2. Beloglazov, G. S., Sikachina, A. A., & Beloglazov, S. M. (2014). Modelling macroscopic properties of organic species on the basis of quantum chemical analysis (on an example of inhibiting efficiency of ureides and acetylides against corrosion). *Solid State Phenomena*, 225, 7–12. doi:10.4028/www.scientific.net/SSP.225.
3. Myamina, M. A., Beloglazov, S. M., & Gribankova, A. A. (2008). Electrochemical study of action of industrial organic additives at steel with Cd-coating by microbial (SRB-induced) corrosion in salted aqueous media. *Sviridov Readings 2008: Book of Abstracts of 4-th International Conference on Chemical Education, Minsk, Krasico-Print*, 40.
4. Al-Amiery, A. A., Kadhum, A. A. H., Alobaidy, A. H. M., Mohamad, A. B., & Hoon, P. S. (2014). Novel Corrosion Inhibitor for Mild Steel in HCl. *Materials*, (7), 662–672. doi:10.3390/ma7020662.
5. Asegbeloyin, J. N., Ejikeme, P. M., Olasunkanmi, L. O., Adekunle, A. S., & Ebenso, E. E. (2015). A Novel Schiff Base of 3-acetyl-4-hydroxy-6-methyl-(2H)pyran-2-one and 2,2'-(ethylenedioxy)diethylamine as Potential Corrosion Inhibitor for Mild Steel in Acidic Medium. *Materials*, (8), 2918–2934. doi:10.3390/ma8062918.
6. Dibetsoe, M., Olasunkanmi, L. O., Fayemi, O. E., Yesudass, S., Ramaganthan, B., Bahadur, I., Adekunle, A. S., Kabanda, M. M., & Ebenso, E. E. (2015). Some Phthalocyanine and Naphthalocyanine Derivatives as Corrosion Inhibitors for Aluminium in Acidic Medium: Experimental, Quantum Chemical Calculations, QSAR Studies and Synergistic Effect of Iodide Ions. *Molecules*, 20, 15701–15734. doi:10.3390/molecules200915701.
7. Kadhum, A. A. H., Mohamad, A. B., Hamed, L. A., Al-Amiery, A. A., San, N. H., & Musa, A. Y. (2014). Inhibition of Mild Steel Corrosion in Hydrochloric Acid Solution by New Coumarin. *Materials*, (7), 4335–4348. doi:10.3390/ma7064335.
8. Mashuga, M. E., Olasunkanmi, L. O., Adekunle, A. S., Yesudass, S., Kabanda, M. M., & Ebenso, E. E. (2015). Adsorption, Thermodynamic and Quantum Chemical Studies of 1-hexyl-3-methylimidazolium Based Ionic Liquids as Corrosion Inhibitors for Mild Steel in HCl. *Materials*, (8), 3607–3632. doi:10.3390/ma8063607.
9. Eddy, N. O., Momoh–Yahaya, H., & Oguzie, E. E. (2015). Theoretical and experimental studies on the corrosion inhibition potentials of some purines for aluminum in 0.1 M HCl. *Journal of Advanced Research*, 6, (2), 203–217. doi:10.1016/j.jare.2014.01.004.
10. Peme, T., Olasunkanmi, L. O., Bahadur, I., Adekunle, A. S., Kabanda, M. M., & Ebenso, E. E. (2015). Adsorption and Corrosion Inhibition Studies of Some Selected Dyes as Corrosion Inhibitors for Mild Steel in Acidic Medium: Gravimetric, Electrochemical, Quantum Chemical Studies and Synergistic Effect with Iodide Ions. *Molecules*, 20, 16004–16029. doi:10.3390/molecules200916004.
11. Singh, A., Lin, Y., Quraishi, M. A., Olasunkanmi, L. O., Fayemi, O. E., Sasikumar, Y., Ramaganthan, B., Bahadur, I., Obot, I. B., Adekunle, A. S., Kabanda, M. M., & Ebenso, E. E.

(2015). Porphyrins as Corrosion Inhibitors for N80 Steel in 3.5% NaCl Solution: Electrochemical, Quantum Chemical, QSAR and Monte Carlo Simulations Studies. *Molecules*, 20, 15122–15146. doi:10.3390/molecules200815122.

12. Sikachina, A. A. (2015). Brief materials on a particular aspect of the study inhibitory activity of organic compounds. *Abstracts of the 69th International Youth Scientific Conference “Oil and Gas — 2015”*. Moscow, 2, 235. Available at: <http://smno.gubkin.ru/doc/2015Tezisy2.pdf>.

13. Geerlings, P., & De Proft, F. (2002). Chemical Reactivity as Described by Quantum Chemical Methods. *Int. J. Mol. Sci.*, (3), 276–309. doi:10.3390/i3040276.

14. Junaedi, S., Al-Amiery, A. A., Kadhim, A., Kadhum, A. A. H., & Mohamad, A. B. (2013). Inhibition Effects of a Synthesized Novel 4-Aminoantipyrine Derivative on the Corrosion of Mild Steel in Hydrochloric Acid Solution together with Quantum Chemical Studies. *Int. J. Mol. Sci.*, 14, 11915–11928. doi:10.3390/ijms140611915.

15. Saranya, J., Sounthari, P., Kiruthika, A., Saranya, G., Yuvarani, S., Parameswari, K., & Chitra, S. (2014). Experimental and Quantum chemical studies on the inhibition potential of some Quinoxaline derivatives for mild steel in acid media. *Orient J Chem*, 30, (4). Available at: <http://www.orientjchem.org/?p=5335>.

16. Zilberberg, I., Pelmenschikov, A., Mcgrath, C. J., Davis, W., Leszczynska, D., & Leszczynski, J. (2002). Reduction of Nitroaromatic Compounds on the Surface of Metallic Iron: Quantum Chemical Study. *Int. J. Mol. Sci.*, (3), 801–813. doi:10.3390/i3070801.

17. Sikachina, A. A. (2015). Quantum chemical modeling of the adsorption of organic compounds on steel carbon structural. *Internet-journal “Naukovedenie”*, 7, (4), doi:10.15862/47TVN415.

18. Ebenso, E. E., Isabirye, D. A., & Eddy, N. O. (2010). Adsorption and Quantum Chemical Studies on the Inhibition Potentials of Some Thiosemicarbazides for the Corrosion of Mild Steel in Acidic Medium. *Int. J. Mol. Sci.*, 11, 2473–2498. doi:10.3390/ijms11062473.

19. Reutov, O. A., Kurtz, A. L., & Butin, K. P. (2010). Organic Chemistry. 3rd ed. Moscow, MSU, Knowledge Laboratory, 1, 700.

20. Ramkumar, S., Nalini, D. (2015). Correlation between inhibition efficiency and chemical structure of new indoloimidazoline on the corrosion of mild steel in molar HCl with DFT evidences. *Orient J Chem*, 31, (2).

21. Sikachina, A. (2016). Quantum chemical modeling of adsorption of ureides, that used as inhibitor of microbiological corrosion, on the iron of st3s grade of steel. *DOAJ — Lund University: Konzept: Scientific and Methodological e-magazine*, (5). Available at: <http://www.doaj.net/10322/>.

#### Список литературы:

1. Iyer R. N., Pickering H. W., Takeuchi I., Zamanzadeh H. Hydrogen Sulfide Effect on Hydrogen Entry into Iron. A Mechanistic Study // *Corrosion*. 1990. V. 46. №6. P. 460–467.

2. Beloglazov G. S., Sikachina A. A., Beloglazov S. M. Modelling macroscopic properties of organic species on the basis of quantum chemical analysis (on an example of inhibiting efficiency of ureides and acetylides against corrosion) // *Solid State Phenomena*. 2014. V. 225. P. 7–12. DOI: 10.4028/www.scientific.net/SSP.225.

3. Myamina M. A., Beloglazov S. M., Gribankova A. A. Electrochemical study of action of industrial organic additives at steel with Cd-coating by microbial (SRB-induced) corrosion in salted aqueous media // *Sviridov Readings 2008: Book of Abstracts of 4-th International Conference on Chemical Education*. Minsk: Krasico-Print, 2008. P. 40.

4. Al-Amiery A. A., Kadhum A. A. H., Alobaidy, A. H. M., Mohamad A. B., Hoon P. S. Novel Corrosion Inhibitor for Mild Steel in HCl // *Materials*. 2014. №7. P. 662–672. DOI: 10.3390/ma7020662.

5. Asegbeloyin J. N., Ejikeme P. M., Olasunkanmi L. O., Adekunle A. S., Ebenso E. E. A Novel Schiff Base of 3-acetyl-4-hydroxy-6-methyl-(2H)pyran-2-one and 2,2'-

(ethylenedioxy)diethylamine as Potential Corrosion Inhibitor for Mild Steel in Acidic Medium // Materials. 2015. №8. P. 2918–2934. DOI: 10.3390/ma8062918.

6. Dibetsoe M., Olasunkanmi L. O., Fayemi O. E., Yesudass S., Ramaganthan B., Bahadur I., Adekunle A. S., Kabanda M. M., Ebenso E. E. Some Phthalocyanine and Naphthalocyanine Derivatives as Corrosion Inhibitors for Aluminium in Acidic Medium: Experimental, Quantum Chemical Calculations, QSAR Studies and Synergistic Effect of Iodide Ions // Molecules. 2015. №20. P. 15701–15734. DOI: 10.3390/molecules200915701.

7. Kadhum A. A. H., Mohamad A. B., Hammed L. A., Al-Amiery A. A., San N. H., Musa A. Y. Inhibition of Mild Steel Corrosion in Hydrochloric Acid Solution by New Coumarin // Materials. 2014. №7. P. 4335–4348. DOI: 10.3390/ma7064335.

8. Mashuga M. E., Olasunkanmi L. O., Adekunle A. S., Yesudass S., Kabanda M. M., Ebenso E. E. Adsorption, Thermodynamic and Quantum Chemical Studies of 1-hexyl-3-methylimidazolium Based Ionic Liquids as Corrosion Inhibitors for Mild Steel in HCl // Materials. 2015. №8. P. 3607–3632. DOI: 10.3390/ma8063607.

9. Eddy N. O., Momoh–Yahaya H., Oguzie E. E. Theoretical and experimental studies on the corrosion inhibition potentials of some purines for aluminum in 0.1 M HCl // Journal of Advanced Research. 2015. V. 6. №2. P. 203–217. DOI: 10.1016/j.jare.2014.01.004.

10. Peme T., Olasunkanmi L. O., Bahadur I., Adekunle A. S., Kabanda M. M., Ebenso E. E. Adsorption and Corrosion Inhibition Studies of Some Selected Dyes as Corrosion Inhibitors for Mild Steel in Acidic Medium: Gravimetric, Electrochemical, Quantum Chemical Studies and Synergistic Effect with Iodide Ions // Molecules. 2015. №20. P. 16004–16029. DOI: 10.3390/molecules200916004.

11. Singh A., Lin Y., Quraishi M. A., Olasunkanmi L. O., Fayemi O. E., Sasikumar Y., Ramaganthan B., Bahadur I., Obot I. B., Adekunle A. S., Kabanda M. M., Ebenso E. E. Porphyrins as Corrosion Inhibitors for N80 Steel in 3.5% NaCl Solution: Electrochemical, Quantum Chemical, QSAR and Monte Carlo Simulations Studies // Molecules. 2015. №20, P. 15122–15146. DOI: 10.3390/molecules200815122.

12. Сикачина А. А. Краткие материалы по конкретному аспекту исследования ингибиторной активности органических соединений // 69-ая международная молодежная научная конференция «Нефть и газ — 2015» (14–16 апреля 2015 г.): сборник тезисов. Т. 2. М.: РГУ нефти и газа им. И. М. Губкина, 2015. С. 235. Режим доступа: <http://smno.gubkin.ru/doc/2015Tezisy2.pdf>.

13. Geerlings P., De Proft F. Chemical Reactivity as Described by Quantum Chemical Methods // Int. J. Mol. Sci. 2002. №3. P. 276–309. DOI: 10.3390/i3040276.

14. Junaedi S., Al-Amiery A. A., Kadhum A., Kadhum A. A. H., Mohamad A. B. Inhibition Effects of a Synthesized Novel 4-Aminoantipyrine Derivative on the Corrosion of Mild Steel in Hydrochloric Acid Solution together with Quantum Chemical Studies // Int. J. Mol. Sci. 2013. №14. P. 11915–11928. DOI: 10.3390/ijms140611915.

15. Saranya J., Sounthari P., Kiruthika A., Saranya G., Yuvarani S., Parameswari K., Chitra S. Experimental and Quantum chemical studies on the inhibition potential of some Quinoxaline derivatives for mild steel in acid media // Orient J Chem. 2014. V. 30. №4. Режим доступа: <http://www.orientjchem.org/?p=5335>.

16. Zilberberg, I.; Pelmeshnikov, A.; McGrath, C.J.; Davis, W.; Leszczynska, D.; Leszczynski, J. Reduction of Nitroaromatic Compounds on the Surface of Metallic Iron: Quantum Chemical Study // Int. J. Mol. Sci. 2002. №3. P. 801–813. DOI: 10.3390/i3070801.

17. Сикачина А. А. Квантовохимическое моделирование адсорбции органических соединений на стали углеродистой конструкционной // Интернет-журнал «Науковедение». 2015. Т. 7. №4. DOI: 10.15862/47TVN415.

18. Ebenso E. E., Isabirye D. A., Eddy N. O. Adsorption and Quantum Chemical Studies on the Inhibition Potentials of Some Thiosemicarbazides for the Corrosion of Mild Steel in Acidic Medium // Int. J. Mol. Sci. 2010. №11. P. 2473–2498. DOI: 10.3390/ijms11062473.

19. Реутов О. А., Курц А. Л., Бутин К. П. Органическая химия. Изд. 3-е. М: МГУ, Лаборатория знаний, 2010. Т. 1. 700 с.

20. Ramkumar S., Nalini D. Correlation between inhibition efficiency and chemical structure of new indoloimidazoline on the corrosion of mild steel in molar HCl with DFT evidences // *Orient J Chem*. 2015. V. 31. №2.

21. Sikachina A. Quantum chemical modeling of adsorption of ureides, that used as inhibitor of microbiological corrosion, on the iron of st3s grade of steel // *DOAJ — Lund University: Konzept: Scientific and Methodological e-magazine*. 2016. №5. Режим доступа: <http://www.doaj.net/10322/>.

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