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dedicated to the 90th birthday of Academician Aleksey Chuiko

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Матеріали Всеукраїнської конференції з міжнародною участю «Хімія, фізика і технологія поверхні», присвяченій 90-річчю від дня народження академіка НАН України О.О. Чуйка – Київ, 2020. – 210 с.

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Збірник містить тези доповідей, які було представлено на конференції. Тематика конференції: теорія хімічної будови та реакційна здатність поверхні твердих тіл; фізико-хімія поверхневих та міжфазних явищ; хімія, фізика та технологія наноматеріалів; медико-біологічні та біохімічні аспекти дослідження високодисперсних матеріалів. Тези доповідей подано в авторській редакції.

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Poster Presentation

1. Theory of Chemical Structure and Reactivity of Solid Surface

1. **Yu.I. Chuyko**, I.V. Khristenko, O.O. Orlova, M.A. Kolosov. **Sorption of metal ions on the surface of silica modified with phosphonoalkyl groups** (*School of Chemistry, V.N. Karazin Kharkiv National University, Ukraine*).
2. **E.M. Demianenko**, A.G. Grebenyuk, V.V. Lobanov, O.S. Karpenko, N.T. Kartel. **A theoretical study on the redox processes on the surface of graphene clusters** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
3. **O.V. Filonenko**, E.M. Demianenko, V.V. Lobanov. **Quantum-chemical modeling of phosphate interaction with hydrated anatase surface** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
4. **Y.O. Gurova**, A.D. Roshal, A.V. Kyrychenko. **Conformation tuning of ortho-POPOP by coordination with alkaline earth metal ions: DFT study** (*Research Institute of Chemistry, V.N. Karazin Kharkiv National University, Ukraine*).
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7. **V.V. Poltavets**, V.F. Vargalyuk, L.V. Shevchenko. **Mangan(II) aquacomplex oxidation by $\bullet O^-$ anion-radical on the electrode surface** (*Oles Honchar Dnipro National University, Ukraine*).
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2. Physical Chemistry of Surface and Interfacial Phenomena

10. **R.H. Amirov**, I.N. Yakovkin, N.V. Petrova, S.V. Sologub, I.V. Bordeniuk. **Fermi surface of H/Mo(110) adsorption system and related peculiarities in magnetoresistance** (*Institute of Physics, NAS of Ukraine, Kyiv*).
11. **A.E Baibara**[1], M.V. Radchenko[1], M.E. Bugaiova[1], Y.N. Bataev[1], A.I. Ievtushenko[1], Y.A. Stelmakh[2], L.A. Krushynskaya[2], H. Przybylinska[3], T. Story[3], A.I. Dmitriev[1]. **Oxygen magnetic properties of the surface for Co nanoparticles** (*[1]Frantsevich Institute for Problems of Material Science, NAS of Ukraine, Kyiv, [2]E.O. Paton Electric Welding Institute, NAS of Ukraine, Kyiv, [3]Institute of Physics, Polish Academy of Sciences, Warsaw*).
12. **D.Yu. Balakin**, N.L. Suprun, L.Yu. Lopandia. **Adsorption interaction of oxygen with Mo(110) surface: dissociation, oxide formation, and corrosion** (*Institute of Physics, NAS of Ukraine, Kyiv*).

Mangan(II) aquacomplex oxidation by $\bullet O^-$ anion-radical on the electrode surface

V.V. Poltavets, V.F. Vargalyuk, L.V. Shevchenko

Oles Honchar Dnipro National University,
72 Gagarin Avenue, Dnipro 49000, Ukraine, verapolt@yahoo.com

As the experimental values for the electrooxidation standard potentials of Mn^{2+} ions as part of various aquacomplexes are mostly larger than water electrooxidation potential or close to it, we have considered the possibility of the mangan aquacomplex oxidation by •O• and •OH radicals that appear at the anode as a result of water decomposition at the potentials ≥ 1÷1.2 V (pH 1÷5). Given the possibility of the adsorbed •OH-radicals dissociation on the positively charged electrode surface, we have also considered the oxidation of Mn^{2+}cations by $\bullet O^-$ anion-radicals.

According to the energy effect values of the oxidation reactions, the oxidative capacity of the considered radicals increases in a series •O•(-95.89 kJ/mol) < •OH(-174.56 kJ/mol)< $\bullet O^-$ (-458.33 kJ/mol). Moreover, as a result of $\bullet O^-$ particle entering a homogeneous aquacomplex, a complex is formed, in which the oxygen atom, due to its interaction with the water molecule, instantly forms two OH particles (based on the results of quantum chemical analysis): $[MnO(H_2O)_5]^+ \rightarrow [Mn(OH)_2(H_2O)_4]^+$.

The most active reagent of all the ones considered by us is $\bullet O^-$ anion-radical. Oxygen atoms together with water molecules on the platinum surface form a polymer structure $PtO\bullet H_2O \leftrightarrow Pt(OH)_2$ (by the spectral study) that is basically equal to the adsorption layer of OH-radicals. In this structure the bond Pt – O is covalent, and $O^{-\cdots}H^+$ is ionic. In such a structure at $\varphi_{q\leq 0}$ the protons will be held near the chemisorbed $\bullet O^-$ particles, thus shielding them from a direct attack by Mn^{2+} aquacomplexes, whereas at $\varphi_{q>0}$ the protons, repelled from the electrode, provide access to the $\bullet O^-$ radicals (Fig.).

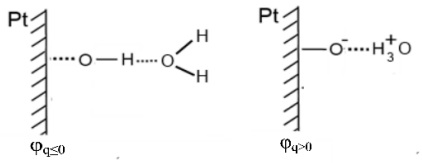

Fig. Model of the •OH-radicals adsorption layer structure on a platinum electrode

Thus, when the charge of the electrode is sufficient for •OH-radicals dissociation, a fast process of $Mn^{2+} + \bullet O^- = MnO^+$ (solutions with pH < 3.0) is started.