

Editorial

Electrocatalytic Activity of Nanocomposites Containing Carbon Materials

Vera Bogdanovskaya *  and Inna VernigorA.N. Frumkin Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences,
119071 Moscow, Russia

* Correspondence: bogd@elchem.ac.ru

Carbon materials (CM), including various allotropic forms of carbon, such as graphene, nanotubes, fullerenes, and other porous structures, are widely used in the synthesis of catalysts. The increased interest in these materials is due to their unique properties such as high stability and electrical conductivity, and the ability to change the electronic structure of these materials by modifying the surface. The high electrical conductivity of CMs makes them practically indispensable in the creation of electrocatalysts for current-forming reactions in current sources. The wide application of CMs for practical purposes requires fundamental research to establish the relationship between their properties and structure, activity, and selectivity with respect to various reactions, both as CMs themselves and as carriers of the metal phase in catalysts. This Special Issue contains articles that contribute both to the development of fundamental concepts that characterize various CMs, their areas of application, and various methods for the synthesis of catalysts. One promising CM is nanotubes, which are characterized by high porosity and increased resistance to degradation. As a result, carbon materials are used to obtain nanocomposite materials of various compositions, which find practical application as independent electrode materials and as carriers of metal nanoparticles, in sensors and other electrochemical applications.

This Special Issue contains 10 research articles.

In [1], using DFT theory, electrodes made of carbon paste modified with asparagine (ASP) and glutamine (GLU) (both environmentally friendly modifiers), differing only in one methyl group, were considered to compare their electrocatalytic abilities and to predict the redox sites of ASP and GLU molecules using computer simulation based on DFT. The electrocatalytic activities of asparagine are higher than those of glutamine for dopamine sensing. Dopamine requires less energy to bind with asparagine when compared to glutamine. Additionally, asparagine has higher electron-donating and accepting powers. Computer modeling using DFT allowed for the redox reactive sites and the mediating mechanisms of the ASP and GLU molecules to be predicted. Thus, in this work, using the example of dopamine determination, the possibility of using quantum chemical calculation methods to predict the sensitivity of modified paste electrodes (MPE) for sensing applications is shown.

In [2], the activity of activated nanocarbon doped with nitrogen, which was synthesized by chemical activation using charcoal as a raw material, was studied. The activity in ORR of this CM is comparable to that of commercial 20% Pt/C catalysts, which may be associated with a highly developed surface area, a favorable ratio and balance of micro- and mesopores, a high content of pyridine nitrogen, and the absence of defects in graphene layers.

It has been established [3] that CNT-based catalysts demonstrate the highest activity in ORR compared to graphene oxide and ultrafine diamond as a support. In addition, bimetallic catalysts based on cobalt and palladium phthalocyanine (MWNT-CoPc-Pd) are characterized by higher activity on all carbon supports compared to materials containing copper and palladium.



Citation: Bogdanovskaya, V.; Vernigor, I. Electrocatalytic Activity of Nanocomposites Containing Carbon Materials. *Catalysts* **2023**, *13*, 370. <https://doi.org/10.3390/catal13020370>

Received: 1 February 2023

Accepted: 6 February 2023

Published: 8 February 2023



Copyright: © 2023 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

CNTs doped with nitrogen can be used as independent catalysts in the reaction of oxygen reduction in alkaline electrolytes. In [4], it was shown that the introduction of nitrogen into the structure of CNTs ensures the adsorption of molecular oxygen in an orientation favorable to the breaking of O–O bonds and the efficient reduction of oxygen at an overvoltage close to that observed on platinum catalysts.

Doping of carbon nanotubes (CNTs) with O, N, and P atoms, described in [5] and used as carriers of platinum nanoparticles, makes it possible to synthesize catalysts with an increased platinum surface due to the presence of a large number of active sites and leads to an increase in the activity of catalysts in the ORR. Regularities have been established for determining methods of targeted synthesis of catalysts due to the preliminary treatment of the carrier, which ensures the formation of a sufficient amount of active groups (oxygen- and nitrogen-containing), which are binding centers for metal nanoparticles.

The electrocatalytic activity of nanocomposites based on CMs is described in [6]. In this study, novel Mo catalysts (Mo/CNT) supported on carbon nanotubes were used to detect L-cysteine (L-Cys, LC). Mo/CNT showed good electrocatalytic responses to LC with high sensitivity, stability and selectivity, which was explained by the presence of weak acid sites on the Mo catalyst enhancing the electrooxidation of LC.

The work [7] reports an increase in oxygen reduction activity when using an electrocatalyst based on spinel oxide $\text{Mn}_{0.5}\text{Ni}_{0.5}\text{Co}_2\text{O}_4/\text{C}$ deposited on a carbon support, which the authors attribute to a large surface area ($209.52\text{ m}^2\text{g}^{-1}$) and high porosity of the support material, as well as a high content of oxygen vacancies on the surface of the carbon support and its electrical conductivity, unlike spinel.

It was shown in [8] that graphene embedded in a carbon matrix was used to manufacture a sensitive electrode in an electrochemical sensor for the determination of Zileuton (ZLT), which, with prolonged use and overdose, causes side effects leading to critical conditions in patients. This sensor is of considerable interest for practical applications.

The study of a series of metal oxide–2D nanomaterials from graphite nitride (series of metal-oxide-doped graphitic carbon nitride 2D nanomaterials) as catalysts for the electrochemical reduction of two water-soluble hydroperoxides—hydrogen peroxide and tert-butyl hydroperoxide—is presented in [9], and the electrocatalytic effect of the modified electrode Co-g- C_3N_4 /Nafion for the electrochemical reduction of both hydroperoxides is shown.

A simple and effective method for the synthesis of porous CoS_2 nanowires doped with Se on carbon fiber and the fabrication of electrodes from carbon paste modified by grinding components is described in [10]. Due to the unique porous structure, the obtained Se- CoS_2 NW/CF has more open active sites and stimulates the release of the formed gas bubbles, which contributes to hydrogen evolution and high electrode stability.

In conclusion, the guest editors of the Special Issue “Electrocatalytic Activity of Nanocomposites Containing Carbon Materials” express their gratitude to all authors for preparing articles that prove the importance of ongoing research in the field of electrocatalysis using nanocomposites containing carbon materials. We also thank the reviewers for their hard work. Additionally, we thank the journal *Catalysts* for the great opportunity to produce this Special Issue.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Jayaprakash, G.K.; Swamy, B.E.K.; Flores-Moreno, R.; Pineda-Urbina, K. Theoretical and Cyclic Voltammetric Analysis of Asparagine and Glutamine Electrocatalytic Activities for Dopamine Sensing Applications. *Catalysts* **2023**, *13*, 100. [\[CrossRef\]](#)
2. Volperts, A.; Plavniece, A.; Kaare, K.; Dobeles, G.; Zhurinsk, A.; Kruusenberg, I. Influence of Chemical Activation Temperatures on Nitrogen-Doped Carbon Material Structure, Pore Size Distribution and Oxygen Reduction Reaction Activity. *Catalysts* **2021**, *11*, 1460. [\[CrossRef\]](#)
3. Bulanova, A.V.; Shafigulin, R.V.; Vinogradov, K.Y.; Tokranova, E.O.; Martynenko, E.A.; Vostrikov, S.V.; Podlipnov, V.V. Effect of Modifying Carbon Materials with Metal Phthalocyanines and Palladium on Their Catalytic Activity in ORR. *Catalysts* **2022**, *12*, 1013. [\[CrossRef\]](#)

4. Bogdanovskaya, V.; Vernigor, I.; Radina, M.; Sobolev, V.; Andreev, V.; Nikolskaya, N. Modified Carbon Nanotubes: Surface Properties and Activity in Oxygen Reduction Reaction. *Catalysts* **2021**, *11*, 1354. [[CrossRef](#)]
5. Bogdanovskaya, V.; Vernigor, I.; Radina, M.; Andreev, V.; Korchagin, O. Nanocomposite Cathode Catalysts Containing Platinum Deposited on Carbon Nanotubes Modified by O, N, and P Atoms. *Catalysts* **2021**, *11*, 335. [[CrossRef](#)]
6. Selçuk, K.; Kivrak, H.; Aktaş, N. Novel CNT Supported Molybdenum Catalyst for Detection of L-Cysteine in Its Natural Environment. *Catalysts* **2021**, *11*, 1561. [[CrossRef](#)]
7. Matthews, T.; Dolla, T.H.; Gwebu, S.S.; Mashola, T.A.; Dlamini, L.T.; Carleschi, E.; Ndungu, P.; Maxakato, N.W. Mn-Ni-Co-O Spinel Oxides towards Oxygen Reduction Reaction in Alkaline Medium: $\text{Mn}_{0.5}\text{Ni}_{0.5}\text{Co}_2\text{O}_4/\text{C}$ Synergism and Cooperation. *Catalysts* **2021**, *11*, 1059. [[CrossRef](#)]
8. Shanbhag, Y.M.; Shanbhag, M.M.; Malode, S.J.; Dhanalakshmi, S.; Mondal, K.; Shetti, N.P. 2D Graphene Sheets as a Sensing Material for the Electroanalysis of Zileuton. *Catalysts* **2022**, *12*, 867. [[CrossRef](#)]
9. Pimpilova, M.; Ivanova-Kolcheva, V.; Stoyanova, M.; Dimcheva, N. 2D Nanomaterial—Based Electrocatalyst for Water Soluble Hydroperoxide Reduction. *Catalysts* **2022**, *12*, 807. [[CrossRef](#)]
10. Tan, Y.; Yin, Y.; Yin, X.; Lan, C.; Wang, Y.; Hu, F.; Huang, Q.; Mi, Y. A “Superaerophobic” Se-Doped CoS_2 Porous Nanowires Array for Cost-Saving Hydrogen Evolution. *Catalysts* **2021**, *11*, 169. [[CrossRef](#)]

Disclaimer/Publisher’s Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.