# MATHEMATICAL MODELING OF THE ELECTRON STRUCTURE OF POLYMER MATRIX *PVDF*+$Pb_2(ZrTiO_6)+(SiO_2)_6$ HYBRID MICRO- AND NANOCOMPOSITE

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**ABSTRACT.**

In this paper there have been presented the results of mathematical modeling of the molecular structure of polymer matrix hybrid micro- and nanocomposites materials having three phases: polyvinylidene fluoride (PVDF) molecule, microparticle of $Pb_2(ZrTiO_6)$ piezoelectric and nanoparticle of $(SiO_2)_6$ dielectric ($PVDF + Pb_2(ZrTiO_6) + (SiO_2)_6$) by using of Parameterized Model number 3 (PM3) semi-empirical method. Molecular orbitals energy, potential ionization, the total electronic energy of $PVDF + Pb_2(ZrTiO_6)+(SiO_2)_6$ nanocomposite have been calculated. The theoretical models of $(SiO_2)_n$ nanoparticle, $Pb_2(ZrTiO_6)$ microparticle and polymer matrix of PVDF 2(h-(-chf-chf-)10-h)+$Pb_2(ZrTiO_6)+(SiO_2)_6$ hybrid micro- and nanocomposite are constructed. The results of calculations show that $PVDF+Pb_2(ZrTiO_6)+(SiO_2)_6$ nanocomposite is solid, electrophile, dielectrical and stable material. The wavelength of the radiated photon is $\lambda \approx 578$ nm. The elasticity of $PVDF+Pb_2(ZrTiO_6)+(SiO_2)_6$ nanocomposite is more than twice the elasticity of PVDF polymer. They will find a wide application in radio engineering, electronics, optoelectronics and piezo technic, seismic and acoustic technics.

# PORE SYSTEM IN THE STRUCTURE OF SOLID POROUS BODIES

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**ABSTRACT**

Porous materials are formed from dispersed particles of various shapes. The porous structure of such materials is determined by the shape and nature of the packing of their structural units. As a model for the analysis of the structure of porous materials, model-packing units were selected in the form of spherical particles and fibers. Separately, the pore structure in foam-like regular porous materials was considered. It is shown that the pore volume in such packages grows with the reduction of the coordination number of the packed spherical particles. To study this regularity, an analysis was made of the structural types of crystal lattices of various chemical substances. Examples of such packages are most metallic elements and all inert gases, with the exception of helium. These substances crystallize in simple structural types. All of them can be considered as packing of balls of identical radii. Such regularities are observed strictly up to the coordination number 4. With coordination number 3, a very openwork, loose package is formed. When forming mixed packages, the coordination number can have fractional values. A special group is represented by structures with coordination number <3. For such structures, an analysis was made of possible combinations of mixed structures with coordination numbers 3 and 2. On the basis of the analysis of the porosity data of various types of packages of spherical particles, an empirical relationship is obtained between the binding porosity and the coordination number of the corresponding package: $\alpha = \alpha'_\infty + \frac{B'}{(n - n_0)}$. An analysis of this dependence showed that there is a certain critical value of the average in the structure of the coordination number in the structures of disperse systems. Less than this value, there is no rigid structure of the framework of the material collected from individual particles. Below this coordination

number, the particles are collected only into separate chain structures that are not related to each other, in which the coordination number 2. The task of analyzing the packing of fibrous particles is much more complicated than this analysis for spherical particles. The article presents data of computer modeling of the formation of such structures. An attempt was also made to model fibrous structures by analogy with an openwork packing of spherical particles. For such and other packing models, the corresponding empirical dependencies. Gel-like materials are characterized by openwork packing of particles forming a gel. They have a fractal and hierarchical nature of the structure. The value of the fractal dimension allows one to determine how the structure of the gel was organized. Analysis of the formation of possible structures in the sol-gel transition showed there is a limiting fractal dimension above which no other structure can be formed from a sol with given properties. This fractal dimension is the amount to which it tends to form a gel structure during the aggregation of the sol, and during the formation of the gel structure, after passing through the sol-gel transition point. An analysis is made of the structure of foam-like regular porous materials. This analysis showed that the state of foam with polyhedral cells is close to the equilibrium state, so these foams have greater stability than foams with spherical cells. Therefore, for the convenience of description, a cellular model based on existing regular polyhedra was applied to these materials. Because of this model, the dependence of the fraction of the solid phase in a porous foam-like solid material, constructed on the basis of cells having the form of various regular polyhedra. The densest structures are formed in the case of using tetrahedral and octahedral cells. The intermediate position is occupied by cubic cells representing a regular three-dimensional network of regular mutually perpendicular columns and bridges.

## THE MAIN WAYS OF CREATING POROUS COMPOSITE MATERIALS

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### ABSTRACT

This paper is devoted to an overview of the main ways of creating porous composite materials. Porous materials are solids containing free space in the form of cavities, channels or pores, which determine the presence of an internal interfacial surface. One of the main characteristics of porous materials is their bulk porosity and specific surface area of the pore space in the material. The paper presents the definitions of these parameters and provides an overview of the main methods for their measurement. The analysis of the general methods of obtaining porous materials. A deposition is one of the most common methods for producing porous materials. Thermal decomposition, as a method used to obtain oxide porous materials by thermal decomposition of various compounds. Hydrothermal synthesis is widely used to produce zeolites. Selective dissolution of individual components of a substance using chemical reactions is also one of the effective methods for creating or increasing porosity. The burning of the combustible component of hydrogels of various hydroxides is also used to form the porosity of some sorption materials. A review of the main methods of obtaining raw materials in the production of porous inorganic composite materials. To date, various methods have been developed for producing microspheres and fibers from materials such as feedstock in the preparation of porous materials. The paper discusses the methods of forming highly porous refractory materials. There are two main ways of forming refractory ceramic products. The first way is direct sintering of dispersions of ceramic fibers. The second method is the use of a binder, which can significantly reduce the temperature of the process of obtaining a porous product. The possibilities of obtaining porous nanocomposites based on aerogels are shown. Composite materials are usually obtained by combining two different materials. In general, the creation of composites is used to take advantage of each type of material, and to minimize their disadvantages. Aerogels are fragile substances. But with the introduction of another component into their structure, it is possible to increase the strength of the material. Such materials have the desired optical properties, high surface area, and low density like silica aerogel. A review of methods for obtaining porous materials using the

phenomenon of spinodal decomposition has been carried out. Materials whose structure is formed in the process of microphase separation during polymerization or polycondensation have high permeability and a sufficiently large specific surface. A significant advantage of such materials is high porosity, which can reach 80% or more.

## TECHNOLOGICAL CAPABILITIES OF LITHIUM EXTRACTION FROM ASSOCIATED OIL BRINES

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**ABSTRACT**

In this article we tried to estimate the size of such mineral resources as underground brines with a low content of lithium. Due to the possible depletion of existing mineral sources of lithium, poor resources may become its most promising resource. This article presents possible directions and prospects for the extraction of lithium from poor sources of raw materials, which are underground brined and associated oil waters. We continued the search for possible solutions to these problems. Nowadays, hydro-mineral raw materials gradually become the main source of lithium. In view of the complexity of the salt composition of hydro-mineral raw materials, the use of highly selective inorganic ion-exchange materials is the most promising method for recovery of lithium**.**

## HIGH-ALTITUDE WIND PLANTS

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**ABSTRACT**

The improvement and implementation of high-altitude wind plants will make it possible to obtain a significant contribution of alternative energy sources to the overall energy balance of the country.