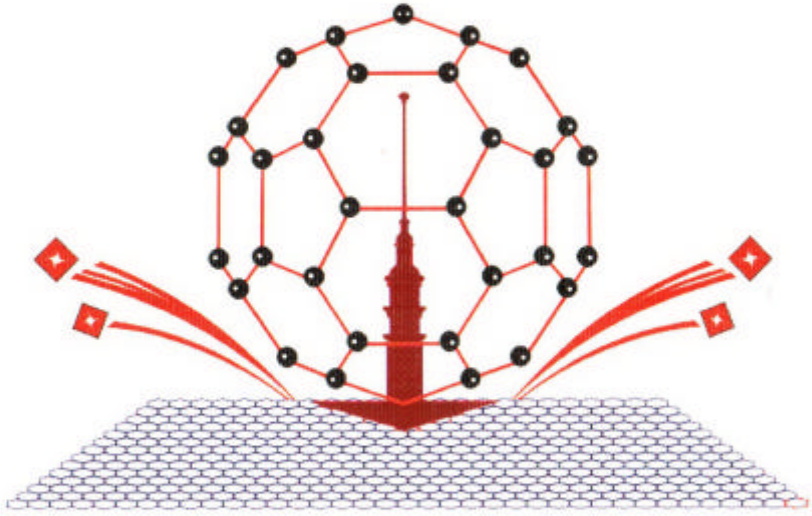
Book of Abstracts

International Conference Advanced Carbon Nanostructures



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Research of hydrogenation of carbon nano-crystalline materials based on pyrolyzed polyacrylonitrile

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For the development of electronics based on nanotechnology are used the new materials of carbon nanocrystalline materials and metal-carbon nanocomposites which in nanoscale are dispersions of inorganic substances in the carbon matrix and revealing large opportunities to controlled obtaining of favorable physico-chemical properties for various applications. The needs of modern industry have stimulated interest in the synthesis of new carbon materials with modified chemical properties based on pyrolyzed polyacrylonitrile (PPAN). Currently a large number of experimental studies of PPAN were made, but not all of them are theoretically justified. This research is devoted to the theoretical study of the mechanism of adsorption of atomic and molecular hydrogen on the surface of the pyrolyzed polyacrylonitrile to determine the properties of the obtained system based on PPAN, which would be useful for a variety of applications.

Studies of adsorption of atomic and molecular hydrogen on the surface of single-and double-layer PPAN on various of atomic composition of the PPAN hexagons have been made. Found that the N atom is negatively effects on the adsorption of atomic H. This is reflected in the reduction of the energy of adsorption in comparison with the case when the H atom attached to the C atom of the surface that does not have the nitrogen atoms in the immediate environment. Performed studies showed that the adsorption of molecules of hydrogen depends on the original position of the molecule relative to the surface of PPAN. Can be implemented, both chemical and physical adsorption. Analysis of the results showed that the nitrogen atom, which is part of the hexagon surface of PPAN, stimulates the process of adsorption of hydrogen molecules.

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Research of adsorption of carbon nanostructures on the base of pyrolized polyacrylonitrile

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The development of science leads to a decrease in the size of the objects of study to the nanometer scale and the creation of physical and chemical methods to produce nanostructures with modified physical and chemical properties that require fundamental and applied research. The needs of modern industry have stimulated interest in the synthesis of new carbon nanocrystalline materials with modified chemical properties based on pyrolyzed polyacrylonitrile. You are currently a large number of experimental studies PPAN, but not all of them are theoretically justified. We studied the mechanism of adsorption of simple gas-phase H, O, F, Cl atoms on the surface of the pyrolyzed polyacrylonitrile. As the object of investigation, the monolayer PPAN containing, in addition to carbon, 20% of the nitrogen atoms of the surface (of the total number of atoms). The distance between the atoms in the layer is 1.4 Å. The study found that the N atom of a negative effect on the adsorption of H and Cl, resulting in a reduction of the energy of adsorption compared to the case when the H atom attached to the C atom of the surface that does not have in the immediate environment of the nitrogen atoms. At the same time, the nitrogen atoms PPAN activate oxidation process and do not affect the process of fluoridation. Found that multiple adsorption of the O atoms on the surface of the monolayer PPAN leads to its destruction when the number of oxygen atoms 10% of the total number of atoms, which is in agreement with the available experimental data on the oxidation of polyacrylonitrile. Increasing the number of nitrogen atoms in the structure PPAN positive impact on the process of oxidation, increasing the maximum number of oxygen atoms adsorbed on the surface of the monolayer without destroying it. Accession of oxygen leads to a curvature of the monolayer planar structure, which may lead to the formation of tubular structures based PPAN. Analysis of the electronic spectra showed a decrease of the band gap oxides PPAN that indicates a change in the conductivity of the adsorption complex towards metallizatsii.Vpervye studied the characteristics of adsorption of H and O atoms on one surface of a two-layer PPAN (symmetric and offset layers on 1 \ 2 hexes). It was found that in all cases originally selected by the physical adsorption of atoms (metastable state), after overcoming a small potential barrier system goes into steady chemisorbed state.

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