

**THE PERFORMANCE OF THE 6-31G^{##} BASIS SET AND ITS MODIFICATIONS
FOR DFT CALCULATION OF NUCLEAR MAGNETIC SHIELDING
AND SPIN-SPIN COUPLING CONSTANTS**

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ABSTRACT

The application of the 6-31G^{##} basis set (recently developed¹ and implemented [2, 3]) for enhancement of the quality of calculations of the nuclear magnetic shielding and indirect nuclear spin–spin coupling constants using the B3LYP hybrid density functional theory is reported. The tested applications include several hydrides, hydrocarbons, fluorinated derivatives of methane and molecules with multiple bonds. For calculations of spin-spin coupling constants the recontraction of functions included in the 6-31G^{##} basis set improves its performance in different molecular space regions. The type of basis functions that should be recontracted depends on the mechanism of coupling. The calculated values of magnetic shielding and indirect nuclear spin–spin coupling constants for all of the systems considered were found to be in good agreement with the results of other theoretical approaches and available experimental data.

ECOLOGICAL PURE SOLAR SILICON TECHNOLOGY

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ABSTRACT

The new carbothermal technology of silicon SoG-Si production reducing of summury harmful pollutions in 50 times is suggested

**ORGANIC-SILICON SENSORS AND RISK ASSESSMENT
OF ORGANIC NANOMATERIAL**

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ABSTRACT

In the paper the various aspects of modern nanobiotechnologies risks impact on an environment, ethical and social issues in nanobiotechnologies are considered. The assessment methods of the individual and social potential risks of nanobiotechnologies (production of organic nano-materials) are considered. With the progress of nanotechnologies the interaction of silicon-based devices with living organisms could be more and more complicated and dangerous. For decreasing environmental risks of nanotechnologies we have developed nano-composite devices based on hybrid organic-silicon matrix. The extended high-resistance organic-silicon sensors have been developed on special matrix technology on the basis of nano-composite materials for measurement both temperature of surrounding sea water, and direction of a stream. Signals from the sensor, amplified of the operational amplifier, by dint of the interface input into a computer for the further processing results of measurement and archiving of the data. Such kind of nano-composite nano-sensors based on hybrid organic-silicon matrix also can be implanted in the body to monitor a range of biological indicators for disease, such as blood sugar levels in diabetics or for measurement of blood flow. The risk assessment of organic nano-materials production is carried out.

ENTROPY PRINCIPLE MAXIMUM FOR HIERARCHICAL DYNAMIC SYSTEMS AND THE TURBULENCE PROBLEM

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ABSTRACT

The entropy principle maximum (or minimum information) is used to derive the equations of the motion for the phase distribution as constraints on the variation problem. This principle survived practically unchanged the upheaval in fluid mechanics, thermodynamics, chemical physics, solid state, nuclear physics, biology, mathematical models for population dynamics. The classical Liouville equation is derived when the constraint is the first order linear differential equation. Maximum entropy replaces the fundamental postulates represented by Newton's laws. The new approach opens the possibility to derive more advanced equations of motion by removing constraints. The entropy principle maximum is developed for a turbulence problem determined by hierarchical dynamical systems. This concept represents the third additional condition which gives possibility to limit the class functions defined the tensor of the transitions between trajectories in the hierarchical equations. The analytical solution is found to Fokker-Planck equation based on the entropy principle maximum for N -dimensional hierarchical dynamical system.

EVALUATION OF THE QUALITY OF CASCADE SEPARATION PROCESSES

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ABSTRACT

Properties and mathematical models of direct and reversed cascade separation processes are examined, which facilitates the correct choice of an apparatus for specific conditions. These models are analyzed in detail, and on their basis the process quality criteria are formulated. Adequacy of these criteria is confirmed by experimental data.