

ISSN 1990-7931

RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY B

Focus on Physics

Editor-in-Chief
Maksim G. Golubkov

Pleiades
Publishing Group
Over **50** years
In the service of
science and education

<https://pleiades.online>
<https://link.springer.com>



PLEIADES GROUP OF COMPANIES

Distributed by **SPRINGER NATURE**

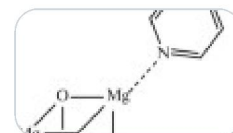


Volume 19, Issue 2
April 2025

ISSN 1070-4280
CODEN RJPCHD

23 articles in this issue

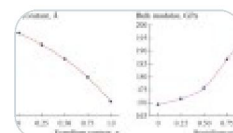
Density Functional Theory Exploring of Substitution and Isotopic Effects on the Adsorption of Pyridine on Mg_4O_4 Cluster



STRUCTURE OF CHEMICAL COMPOUNDS, QUANTUM CHEMISTRY, SPECTROSCOPY
Pages: 271 - 276

08 July 2025

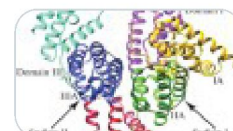
First Principle Investigation by Hybrid Functional Method on the Physical Properties of Narrow Band Gap $Sc_xY_{1-x}N$ ($0 \leq x \leq 1$) Solid Solutions



STRUCTURE OF CHEMICAL COMPOUNDS, QUANTUM CHEMISTRY, SPECTROSCOPY
Pages: 277 - 286

08 July 2025

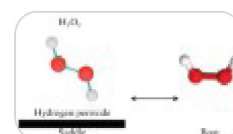
Study on the Interaction of Olmesartan with Human Serum Albumin by Spectroscopic and Molecular Docking Techniques



STRUCTURE OF CHEMICAL COMPOUNDS, QUANTUM CHEMISTRY, SPECTROSCOPY
Pages: 287 - 293

08 July 2025

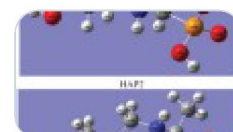
Structure and Properties of Matter—Additive Approach



STRUCTURE OF CHEMICAL COMPOUNDS, QUANTUM CHEMISTRY, SPECTROSCOPY
Pages: 294 - 299

08 July 2025

Synthesis, Density Functional Theory Investigation, Antioxidant and Antibacterial Activities Evaluation of Hydroxybutyl and Hydroxypropyl Aminophosphonic Acids



STRUCTURE OF CHEMICAL COMPOUNDS, QUANTUM CHEMISTRY, SPECTROSCOPY
Pages: 300 - 318

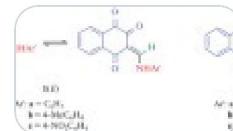
08 July 2025

Divulge of Hydrogen Energy Storage by Manganese Doped Nitrogen Nanocomposites of Aluminum, Gallium or Indium Nitrides: A First-Principles Study



STRUCTURE OF CHEMICAL COMPOUNDS, QUANTUM CHEMISTRY, SPECTROSCOPY | 08 July 2025 |
Pages: 319 - 335

Comparative Study of Electronic Structure and Photophysical Properties of Some New LawsONE Dyes in Dye-Sensitized Solar Cells by DFT and TD-DFT



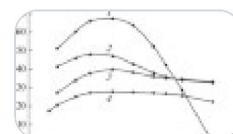
STRUCTURE OF CHEMICAL COMPOUNDS, QUANTUM CHEMISTRY, SPECTROSCOPY | 08 July 2025 |
Pages: 336 - 347

Computational Studies on Maraviroc Derivatives for HIV Treatment: QSAR and Molecular Docking Approaches



STRUCTURE OF CHEMICAL COMPOUNDS, QUANTUM CHEMISTRY, SPECTROSCOPY | 08 July 2025 |
Pages: 348 - 361

The Effect of Temperature on the Cool-Flame Oxidation of Rich Propane-Oxygen Mixtures



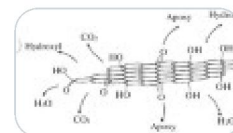
KINETICS AND MECHANISM OF CHEMICAL REACTIONS, CATALYSIS | 08 July 2025 | Pages: 362 - 367

Influence of CTAB and SDS on the Oxidation of Leucine by Quinolinium Dichromate in Presence of HClO_4



KINETICS AND MECHANISM OF CHEMICAL REACTIONS, CATALYSIS | 08 July 2025 | Pages: 368 - 378

Room Temperature Liquefied Petroleum Gas Sensing Based on Reduced Graphene Oxide Thin Film



ELECTRIC AND MAGNETIC PROPERTIES OF CHEMICAL COMPOUNDS | 08 July 2025 | Pages: 379 - 387

Solid-State Lithium-Ion Batteries Based on Using Ionics Conductivity Polymers Interfaces during Interaction between Solid Electrolytes with Both Electrodes



Experimental Study as Well as DFT Calculations for Ion Transport in Hydrogen/Platinum/Iridium Electrode of Fuel Cells through h-BN Layers in Proton Exchange Membrane



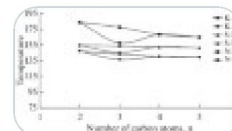
ELECTRIC AND MAGNETIC PROPERTIES OF CHEMICAL COMPOUNDS | 08 July 2025 | Pages: 401 - 416

Experimental and Theoretical Study of metal Doped Dielectric Capacitors Composd with M-GO/(h-BN)_n/M-GO(M = Be, B): A High Capacitance at Micro-Scale



ELECTRIC AND MAGNETIC PROPERTIES OF CHEMICAL COMPOUNDS | 08 July 2025 | Pages: 417 - 431

Thermal Stability of Liquid Crystalline Hydroxamic Acid Derivatives



PHYSICAL METHODS FOR INVESTIGATION OF CHEMICAL PROCESSES | 08 July 2025 | Pages: 432 - 441

Calculations of the Electronic Properties and Absorption of the Carmustine Anticancer Drug Molecule on the Surface of Single-Walled Carbon Nanotubes (8,0) Using Density Functional Theory



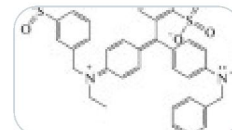
CHEMICAL PHYSICS OF BIOLOGICAL PROCESSES | 08 July 2025 | Pages: 442 - 452

Electrocatalytic Conversion of CO₂ to Formate on a Pb-Graphite Composite Electrode



CHEMICAL PHYSICS OF ECOLOGICAL PROCESSES | 08 July 2025 | Pages: 453 - 465

Polypyrrole-Coated Cobalt Ferrite Nano-Sorbent for Efficient Removal of Fast Green Dye: A Kinetic and Thermodynamic Approach



CHEMICAL PHYSICS OF NANOMATERIALS | 08 July 2025 | Pages: 466 - 479

Unraveling Hetero-Clusters of Indium Gallium Nitride and Its Alloys for Solar Cells Development: Structural and Characterization Study of

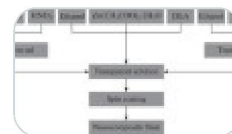
Nitride-Based Semiconductors Using DFT Framework

CHEMICAL PHYSICS OF NANOMATERIALS | 08 July 2025 | Pages: 480 - 500



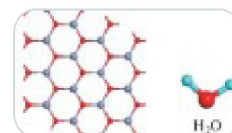
Effects of ZnO-Doping on the Morphology and Mechanical Properties in TiO₂/SiO₂ Nanocomposite Thin Films Via Sol–Gel Process for Coating Application

CHEMICAL PHYSICS OF NANOMATERIALS | 08 July 2025 | Pages: 501 - 506



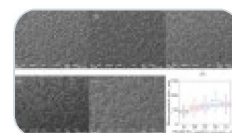
Adsorption of H₂O Molecules Mechanism on Graphene-Like ZnO Monolayer with Promoted Humidity Sensing Performance

REACTIONS ON SURFACE | 08 July 2025 | Pages: 507 - 511



Retardation of Perovskite Crystal Growth by Lead Thiocyanate Addition and Its Effect on Perovskite Solar Cell Performance

REACTIONS ON SURFACE | 08 July 2025 | Pages: 512 - 519



Erratum to: Two-Stage Thermal and Heterogeneous Catalytic Conversion of Hydrolysis Lignin in Supercritical *n*-Hexane

Erratum | 08 July 2025 | Pages: 520 - 520