

ISSN 1990-7931

RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY B

Focus on Physics

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

Editor-in-Chief
Maksim G. Golubkov

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

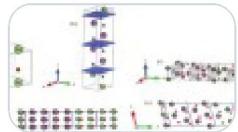


PLEIADES GROUP OF COMPANIES

Distributed by **SPRINGER NATURE**

25 articles in this issue

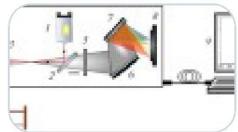
Scandium-Engineered GaN Alloys and Superlattices: Multiscale DFT and SCAPS-1D Design for High-Efficiency Optoelectronic Solar Cells



STRUCTURE OF CHEMICAL COMPOUNDS, QUANTUM CHEMISTRY, SPECTROSCOPY |

29 January 2026 | Pages: 1297 - 1309

Machine Learning Methods for Classification of Organic and Inorganic Compounds Raman Spectra



STRUCTURE OF CHEMICAL COMPOUNDS, QUANTUM CHEMISTRY, SPECTROSCOPY |

29 January 2026 | Pages: 1310 - 1316

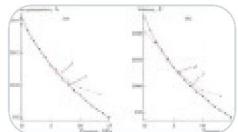
Structural, Electronic and Spin Density Properties of Graphitic Nano-Silicon Carbide as a Recent Anode Electrode for Developed (Li,Na,Be,Mg)-Ion Batteries: A Quantum Computing Study by DFT-D3 Method



STRUCTURE OF CHEMICAL COMPOUNDS, QUANTUM CHEMISTRY, SPECTROSCOPY |

29 January 2026 | Pages: 1317 - 1327

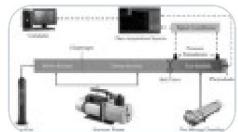
Structural, Electronic, Optical, Elastic Properties of Chiral Semiconductor Ag₃AuTe₂ from First-Principles Calculations



STRUCTURE OF CHEMICAL COMPOUNDS, QUANTUM CHEMISTRY, SPECTROSCOPY |

29 January 2026 | Pages: 1328 - 1337

Experimental Investigation of Auto Ignition of Ethylene and Propulsion Grade Kerosene



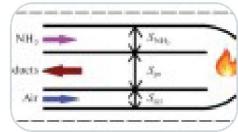
COMBUSTION, EXPLOSION, AND SHOCK WAVES | 29 January 2026 | Pages: 1338 - 1352

Shock Waves during Detonation of Hydrogen–Air Mixture Confined by a Movable Thin-Walled Shell



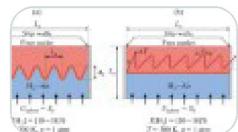
COMBUSTION, EXPLOSION, AND SHOCK WAVES | 29 January 2026 | Pages: 1353 - 1359

Thermodynamic Evaluation of Hydrogen Production Modes during Ammonia Pyrolysis in the Swiss-Roll Reactor



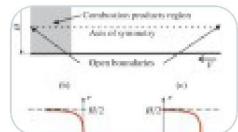
COMBUSTION, EXPLOSION, AND SHOCK WAVES | 29 January 2026 | Pages: 1360 - 1365

Development of Flame Instability Induced by Perturbations of Finite Amplitude in Lean Hydrogen–Air Mixtures



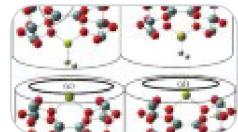
COMBUSTION, EXPLOSION, AND SHOCK WAVES | 29 January 2026 | Pages: 1366 - 1372

Flame Acceleration under Conditions of Boundary Layer Instability Development



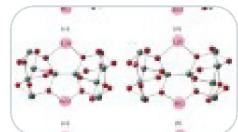
COMBUSTION, EXPLOSION, AND SHOCK WAVES | 29 January 2026 | Pages: 1373 - 1378

Next-Generation Alkaline Earth Metal-Based Batteries and Synergy of Silicon/Germanium/Tin Anode Material: A Quantum Computing Study



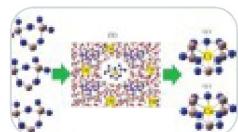
ELECTRIC AND MAGNETIC PROPERTIES OF MATERIALS | 29 January 2026 | Pages: 1379 - 1389

Unlocking Physical Properties of Charge Density and Electron Localization Function of Metal/Metalloid Substitution in Hybrid Semiconductors of Silicon–Germanium Oxide: A DFT Simulation



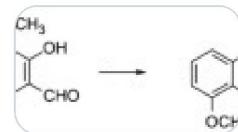
ELECTRIC AND MAGNETIC PROPERTIES OF MATERIALS | 29 January 2026 | Pages: 1390 - 1400

Electromagnetic and Density of States Characterization of Hybrid GaN-Based Nanocomposite for Transition Metals [Cr(III), Co(II), Cu(II), Ni(II)] Removal from Clean Water: A Quantum Study



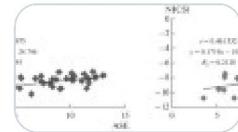
ELECTRIC AND MAGNETIC PROPERTIES OF MATERIALS | 29 January 2026 | Pages: 1401 - 1412

Alternating Current and Direct Current Magnetic Susceptibility Study on a Novel Polydentate Schiff Base (Salen Ligands)–Cerium(III) Complex: Synthesis, Characterization, Thermal, and DFT Studies



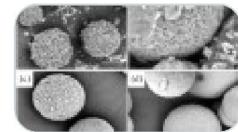
ELECTRIC AND MAGNETIC PROPERTIES OF MATERIALS | 29 January 2026 | Pages: 1413 - 1424

Theoretical Study of the Aromatic Properties and Reactivity of Carbon Atoms in a Group of Five-Membered Heterocycles Containing *N*-Oxide Bonds



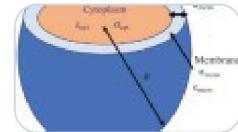
ELECTRIC AND MAGNETIC PROPERTIES OF MATERIALS | 29 January 2026 | Pages: 1425 - 1438

Preparation and Wave Absorption Properties of Urea-Formaldehyde Resin-Based Flower-Like Carbon Microspheres



ELECTRIC AND MAGNETIC PROPERTIES OF MATERIALS | 29 January 2026 | Pages: 1439 - 1447

Electrokinetic-Induced Isolation of Circulating Tumor Cells in a Microfluidic Device under the Influence of External Electric Field: A Computational Study



ELECTRIC AND MAGNETIC PROPERTIES OF MATERIALS | 29 January 2026 | Pages: 1448 - 1457

Strategies for Regulating the Photocatalytic Activity of Sn-Based Materials via Heat Treatment



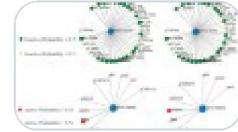
PHYSICAL METHODS FOR INVESTIGATION OF CHEMICAL PROCESSES | 29 January 2026 |
Pages: 1458 - 1465

Photochemistry of Carboranylchlorin and its Complexes with DNA

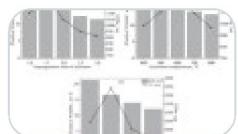


CHEMICAL PHYSICS OF BIOLOGICAL PROCESSES | 29 January 2026 | Pages: 1466 - 1471

Efficient Synthesis, Computational Drug-Likeness, and Molecular Docking Studies of Novel Bicyclic Benzylidene Thiazol[3,2-A]Pyrimidin-3(2H)-One Derivatives for Oncogenic and Neurotherapeutic Targets

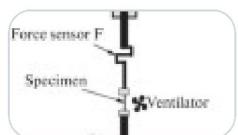


Efficient Removal of Dibenzothiophene from Liquid Oil and Cr(VI) from Waste Water Using Tea Waste-Derived Magnetic Activated Carbon Nanocomposite



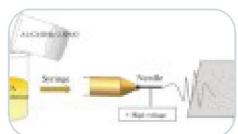
CHEMICAL PHYSICS OF ECOLOGICAL PROCESSES | 29 January 2026 | Pages: 1486 - 1502

Elaboration and Identification of the Physical Properties of Magnetorheological Elastomer



CHEMICAL PHYSICS OF POLYMER MATERIALS | 29 January 2026 | Pages: 1503 - 1513

Relationship between Spinning Aid Polyvinyl Alcohol and Morphology of Alumina Nanofibers via Electrospinning Method



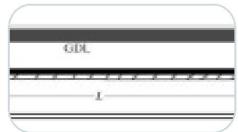
CHEMICAL PHYSICS OF NANOMATERIALS | 29 January 2026 | Pages: 1514 - 1525

Transition Metals-Modified $(\text{BN}_2)_5$ Smart Nanocage for CO/NO Detection: Structural, Electromagnetic and Thermodynamic Properties of Gas Sensors by DFT Quantum Computing



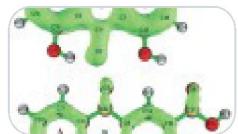
CHEMICAL PHYSICS OF NANOMATERIALS | 29 January 2026 | Pages: 1526 - 1538

Computational Fluid Dynamics for Direct Methanol, Direct Formic Acid, and Alkaline Fuel Cells: Comparison the Net Power with Proton Exchange Membrane Fuel Cells



DYNAMICS OF TRANSPORT PROCESSES | 29 January 2026 | Pages: 1539 - 1550

A Comparative Study of Reaction Sites of Planar Rhein: A density Functional Theory Study



REACTIONS ON SURFACE | 29 January 2026 | Pages: 1551 - 1556