

# Zakhar I Popov

## List of Publications by Year in descending order

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Version: 2024-02-01

67  
papers

1,638  
citations

331670

21  
h-index

315739

38  
g-index

69  
all docs

69  
docs citations

69  
times ranked

3090  
citing authors

#	ARTICLE	IF	CITATIONS
1	Hexagonal BN- and BNO-supported Au and Pt nanocatalysts in carbon monoxide oxidation and carbon dioxide hydrogenation reactions. Applied Catalysis B: Environmental, 2022, 303, 120891.	20.2	26
2	Computational Design of Gas Sensors Based on V3S4 Monolayer. Nanomaterials, 2022, 12, 774.	4.1	7
3	Biodegradable Nanohybrid Materials as Candidates for Self-Sanitizing Filters Aimed at Protection from SARS-CoV-2 in Public Areas. Molecules, 2022, 27, 1333.	3.8	11
4	Raman Spectroscopy of Janus MoSSe Monolayer Polymorph Modifications Using Density Functional Theory. Materials, 2022, 15, 3988.	2.9	6
5	Metastable structures of CaCO <sub>3</sub> and their role in transformation of calcite to aragonite and postaragonite. Crystal Growth and Design, 2021, 21, 65-74.	3.0	16
6	Highly efficient bilateral doping of single-walled carbon nanotubes. Journal of Materials Chemistry C, 2021, 9, 4514-4521.	5.5	17
7	Metallocene inspired 2D metal intercalated carbon allotropes: Stability and properties via DFT calculations. Carbon, 2021, 184, 714-720.	10.3	3
8	Novel two-dimensional boron oxynitride predicted using the USPEX evolutionary algorithm. Physical Chemistry Chemical Physics, 2021, 23, 26178-26184.	2.8	4
9	Electrospun Biodegradable Nanofibers Coated Homogenously by Cu Magnetron Sputtering Exhibit Fast Ion Release. Computational and Experimental Study. Membranes, 2021, 11, 965.	3.0	11
10	Polyol Synthesis of Ag/BN Nanohybrids and their Catalytic Stability in CO Oxidation Reaction. ChemCatChem, 2020, 12, 1691-1698.	3.7	11
11	Adhesion of Single-Walled Carbon Nanotube Thin Films with Different Materials. Journal of Physical Chemistry Letters, 2020, 11, 504-509.	4.6	8
12	Non-chemical fluorination of hexagonal boron nitride by high-energy ion irradiation. Nanotechnology, 2020, 31, 125705.	2.6	5
13	Graphene/Half-Metallic Heusler Alloy: A Novel Heterostructure toward High-Performance Graphene Spintronic Devices. Advanced Materials, 2020, 32, 1905734.	21.0	16
14	Induced spin polarization in graphene <i>via</i> interactions with halogen doped MoS <sub>2</sub> and MoSe <sub>2</sub> monolayers by DFT calculations. Nanoscale, 2020, 12, 23248-23258.	5.6	13
15	Alkali metals inside bi-layer graphene and MoS <sub>2</sub> : Insights from first-principles calculations. Nano Energy, 2020, 75, 104927.	16.0	30
16	Stability and gas sensing properties of Ta <sub>2</sub> X <sub>3</sub> M <sub>8</sub> (X = Pd, Pt; M = S,) Tj ETQq0 0 0 rgBT /Overlock 14651-14659.	2.8	6
17	Exotic Two-Dimensional Structure: The First Case of Hexagonal NaCl. Journal of Physical Chemistry Letters, 2020, 11, 3821-3827.	4.6	38
18	(Ni,Cu)/hexagonal BN nanohybrids " New efficient catalysts for methanol steam reforming and carbon monoxide oxidation. Chemical Engineering Journal, 2020, 395, 125109.	12.7	39

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19	Spintronic Devices: Graphene/Half-Metallic Heusler Alloy: A Novel Heterostructure toward High-Performance Graphene Spintronic Devices (Adv. Mater. 6/2020). Advanced Materials, 2020, 32, 2070043.	21.0	0
20	Transition Metal Chalcogenide Single Layers as an Active Platform for Single-Atom Catalysis. ACS Energy Letters, 2019, 4, 1947-1953.	17.4	43
21	TiCaPCON-Supported Pt- and Fe-Based Nanoparticles and Related Antibacterial Activity. ACS Applied Materials & Interfaces, 2019, 11, 28699-28719.	8.0	16
22	Influence of Native Defects on the Electronic and Magnetic Properties of CVD Grown MoSe <sub>2</sub> Single Layers. Journal of Physical Chemistry C, 2019, 123, 24855-24864.	3.1	22
23	Structural evolution of Ag/BN hybrids via a polyol-assisted fabrication process and their catalytic activity in CO oxidation. Catalysis Science and Technology, 2019, 9, 6460-6470.	4.1	7
24	Al-BN interaction in a high-strength lightweight Al/BN metal-matrix composite: Theoretical modelling and experimental verification. Journal of Alloys and Compounds, 2019, 782, 875-880.	5.5	20
25	Temperature induced twinning in aragonite: transmission electron microscopy experiments and <i>ab initio</i> calculations. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 79-84.	0.8	4
26	Dirac Cone Spin Polarization of Graphene by Magnetic Insulator Proximity Effect Probed with Outermost Surface Spin Spectroscopy. Advanced Functional Materials, 2018, 28, 1800462.	14.9	12
27	Compressive properties of hollow BN nanoparticles: theoretical modeling and testing using a high-resolution transmission electron microscope. Nanoscale, 2018, 10, 8099-8105.	5.6	8
28	Highly conductive and transparent films of HAuCl <sub>4</sub> -doped single-walled carbon nanotubes for flexible applications. Carbon, 2018, 130, 448-457.	10.3	68
29	BN nanoparticle/Ag hybrids with enhanced catalytic activity: theory and experiments. Catalysis Science and Technology, 2018, 8, 1652-1662.	4.1	23
30	Interface-induced perpendicular magnetic anisotropy of Co nanoparticles on single-layer h-BN/Pt(111). Applied Physics Letters, 2018, 112, 022407.	3.3	6
31	Construction of Polarized Carbon-Nickel Catalytic Surfaces for Potent, Durable, and Economic Hydrogen Evolution Reactions. ACS Nano, 2018, 12, 4148-4155.	14.6	121
32	Grafting of carboxyl groups using CO <sub>2</sub> /C <sub>2</sub> H <sub>4</sub> /Ar pulsed plasma: Theoretical modeling and XPS derivatization. Applied Surface Science, 2018, 435, 1220-1227.	6.1	27
33	Synthetic routes, structure and catalytic activity of Ag/BN nanoparticle hybrids toward CO oxidation reaction. Journal of Catalysis, 2018, 368, 217-227.	6.2	18
34	Spontaneous doping of the basal plane of MoS <sub>2</sub> single layers through oxygen substitution under ambient conditions. Nature Chemistry, 2018, 10, 1246-1251.	13.6	295
35	Holey single-walled carbon nanotubes for ultra-fast broadband bolometers. Nanoscale, 2018, 10, 18665-18671.	5.6	29
36	Photocatalysis with Pt-Au-ZnO and Au-ZnO Hybrids: Effect of Charge Accumulation and Discharge Properties of Metal Nanoparticles. Langmuir, 2018, 34, 7334-7345.	3.5	47

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37	Effect of chemical ordering on optical properties of Fe <sub>3</sub> Si epitaxial films. EPJ Web of Conferences, 2018, 185, 03014.	0.3	2
38	Analysis of epoxy functionalized layers synthesized by plasma polymerization of allyl glycidyl ether. Physical Chemistry Chemical Physics, 2018, 20, 20070-20077.	2.8	13
39	High-pressure phases of sulfur: Topological analysis and crystal structure prediction. Physica Status Solidi (B): Basic Research, 2017, 254, 1600857.	1.5	13
40	Multifunctional Superelastic Foam-Like Boron Nitride Nanotubular Cellular-Network Architectures. ACS Nano, 2017, 11, 558-568.	14.6	110
41	VS <sub>2</sub> /Graphene Heterostructures as Promising Anode Material for Li-Ion Batteries. Journal of Physical Chemistry C, 2017, 121, 24179-24184.	3.1	73
42	Aragonite-II and CaCO <sub>3</sub> -VII: New High-Pressure, High-Temperature Polymorphs of CaCO <sub>3</sub> . Crystal Growth and Design, 2017, 17, 6291-6296.	3.0	61
43	Immobilization of Platelet-Rich Plasma onto COOH Plasma-Coated PCL Nanofibers Boost Viability and Proliferation of Human Mesenchymal Stem Cells. Polymers, 2017, 9, 736.	4.5	35
44	Molecular dynamical modelling of endohedral fullerenes formation in plasma. IOP Conference Series: Materials Science and Engineering, 2016, 110, 012078.	0.6	0
45	Toward Analysis of Structural Changes Common for Alkaline Carbonates and Binary Compounds: Prediction of High-Pressure Structures of Li <sub>2</sub> CO <sub>3</sub> , Na <sub>2</sub> CO <sub>3</sub> , and K <sub>2</sub> CO <sub>3</sub> . Crystal Growth and Design, 2016, 16, 5612-5617.	3.0	15
46	Stability of B2-type FeS at Earth's inner core pressures. Geophysical Research Letters, 2016, 43, 8435-8440.	4.0	10
47	Proximity-Induced Spin Polarization of Graphene in Contact with Half-Metallic Manganite. ACS Nano, 2016, 10, 7532-7541.	14.6	44
48	The electronic structure and spin states of 2D graphene/VX <sub>2</sub> (X = S, Se) heterostructures. Physical Chemistry Chemical Physics, 2016, 18, 33047-33052.	2.8	49
49	Analysis of thermal effects on copper nanoparticles synthesized from the gas phase. IOP Conference Series: Materials Science and Engineering, 2015, 81, 012033.	0.6	1
50	Prediction and theoretical investigation of new 2D and 3D periodical structures, having graphene-like bandstructures. Physica Status Solidi (B): Basic Research, 2015, 252, 2407-2411.	1.5	2
51	Theoretical study of $\epsilon$ -Fe <sub>4</sub> N and $\delta$ -Fe <sub>x</sub> N iron nitrides at pressures up to 500 GPa. JETP Letters, 2015, 101, 371-375.	1.4	11
52	Analysis of optical and magneto-optical spectra of Fe <sub>5</sub> Si <sub>3</sub> and Fe <sub>3</sub> Si magnetic silicides using spectral magnetoellipsometry. Journal of Experimental and Theoretical Physics, 2015, 120, 886-893.	0.9	12
53	Ab initio and empirical modeling of lithium atoms penetration into silicon. Computational Materials Science, 2015, 109, 76-83.	3.0	3
54	Unbiased crystal structure prediction of NiSi under high pressure. Journal of Applied Crystallography, 2015, 48, 906-908.	4.5	3

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55	First-principles calculations of the equations of state and relative stability of iron carbides at the Earth's core pressures. Russian Geology and Geophysics, 2015, 56, 164-171.	0.7	12
56	Enhanced electron coherence in atomically thin Nb <sub>3</sub> SiTe <sub>6</sub> . Nature Physics, 2015, 11, 471-476.	16.7	46
57	Phase transformations of Fe <sub>3</sub> N-Fe <sub>4</sub> N iron nitrides at pressures up to 30 GPa studied by in situ X-ray diffractometry. JETP Letters, 2014, 98, 805-808.	1.4	14
58	Optical characteristics of an epitaxial Fe <sub>3</sub> Si/Si(111) iron silicide film. JETP Letters, 2014, 99, 565-569.	1.4	9
59	Theoretical study of sorption and diffusion of lithium atoms on the surface of crystalline silicon and inside it. JETP Letters, 2013, 97, 634-638.	1.4	3
60	DFT investigation of the influence of ordered vacancies on elastic and magnetic properties of graphene and graphene-like SiC and BN structures. Physica Status Solidi (B): Basic Research, 2012, 249, 2549-2552.	1.5	28
61	First principal investigation of Fe- and Li- silicon compounds. Physics Procedia, 2012, 23, 17-20.	1.2	0
62	Theoretical study of the diffusion of lithium in crystalline and amorphous silicon. JETP Letters, 2012, 95, 143-147.	1.4	16
63	Small Size Particles of Different Metal Alloys with Protective Shell for Hydrogen Storage. NATO Science for Peace and Security Series C: Environmental Security, 2011, , 167-175.	0.2	0
64	Mobility of vacancies under deformation and their effect on the elastic properties of graphene. Journal of Experimental and Theoretical Physics, 2011, 112, 820-824.	0.9	17
65	Hydrogenation of the nanopowders that form in a carbon-helium plasma stream during the introduction of Ni and Mg. Journal of Experimental and Theoretical Physics, 2011, 113, 1057-1062.	0.9	1
66	Theoretical Study of the Lithium Diffusion in the Crystalline and Amorphous Silicon as well as on its Surface. Solid State Phenomena, 0, 213, 29-34.	0.3	2
67	Theoretical Investigation of Ni <sub>2</sub> Based Bilayer Heterostructures. Key Engineering Materials, 0, 806, 10-16.	0.4	0