

Danil Bukhvalov

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109 papers	2,311 citations	27 h-index	43 g-index
119 ext. papers	2,962 ext. citations	7 avg, IF	5.55 L-index

#	Paper	IF	Citations
109	Origin of anomalous water permeation through graphene oxide membrane. <i>Nano Letters</i> , 2013 , 13, 3930-3935	11.5	205
108	A Computational Investigation of the Catalytic Properties of Graphene Oxide: Exploring Mechanisms by using DFT Methods. <i>ChemCatChem</i> , 2012 , 4, 1844-1849	5.2	112
107	Metal organic frameworks as sorption media for volatile and semi-volatile organic compounds at ambient conditions. <i>Scientific Reports</i> , 2016 , 6, 27813	4.9	94
106	The influence of chemical reactivity of surface defects on ambient-stable InSe-based nanodevices. <i>Nanoscale</i> , 2016 , 8, 8474-9	7.7	79
105	Liquid-Phase Exfoliated Indium-Selenide Flakes and Their Application in Hydrogen Evolution Reaction. <i>Small</i> , 2018 , 14, e1800749	11	68
104	The sensitive detection of formaldehyde in aqueous media using zirconium-based metal organic frameworks. <i>Sensors and Actuators B: Chemical</i> , 2017 , 241, 938-948	8.5	66
103	Chemical modifications and stability of phosphorene with impurities: a first principles study. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 15209-17	3.6	66
102	Hierarchical ultrathin carbon encapsulating transition metal doped MoP electrocatalysts for efficient and pH-universal hydrogen evolution reaction. <i>Nano Energy</i> , 2020 , 70, 104445	17.1	61
101	Unveiling the Mechanisms Leading to H ₂ Production Promoted by Water Decomposition on Epitaxial Graphene at Room Temperature. <i>ACS Nano</i> , 2016 , 10, 4543-9	16.7	56
100	Amine-Functionalized Metal-Organic Frameworks and Covalent Organic Polymers as Potential Sorbents for Removal of Formaldehyde in Aqueous Phase: Experimental Versus Theoretical Study. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 1426-1439	9.5	51
99	Charge Transfer-Induced Molecular Hole Doping into Thin Film of Metal-Organic Frameworks. <i>ACS Applied Materials & Interfaces</i> , 2015 , 7, 18501-7	9.5	49
98	Modeling of hydrogen and hydroxyl group migration on graphene. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 15367-71	3.6	49
97	Development of Highly Water Stable Graphene Oxide-Based Composites for the Removal of Pharmaceuticals and Personal Care Products. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 2899-2913	3.9	48
96	Water Splitting over Graphene-Based Catalysts: Ab Initio Calculations. <i>ACS Catalysis</i> , 2014 , 4, 2016-2021	13.1	47
95	Evidencing Interfacial Charge Transfer in 2D CdS/2D MXene Schottky Heterojunctions toward High-Efficiency Photocatalytic Hydrogen Production. <i>Solar Rrl</i> , 2021 , 5, 2000414	7.1	46
94	Atomic structure, electronic states, and optical properties of epitaxially grown EGa ₂ O ₃ layers. <i>Superlattices and Microstructures</i> , 2018 , 120, 90-100	2.8	45
93	Tailoring the Surface Chemical Reactivity of Transition-Metal Dichalcogenide PtTe ₂ Crystals. <i>Advanced Functional Materials</i> , 2018 , 28, 1706504	15.6	43

92	Triple Functions of Ni(OH) ₂ on the Surface of WN Nanowires Remarkably Promoting Electrocatalytic Activity in Full Water Splitting. <i>ACS Catalysis</i> , 2020 , 10, 13323-13333	13.1	42
91	The characterization of Co-nanoparticles supported on graphene. <i>RSC Advances</i> , 2015 , 5, 75600-75606	3.7	37
90	Adsorptive removal of an eight-component volatile organic compound mixture by Cu-, Co-, and Zr-metal-organic frameworks: Experimental and theoretical studies. <i>Chemical Engineering Journal</i> , 2020 , 397, 125391	14.7	36
89	The Advent of Indium Selenide: Synthesis, Electronic Properties, Ambient Stability and Applications. <i>Nanomaterials</i> , 2017 , 7,	5.4	35
88	Anisotropic magnetism of graphite irradiated with medium-energy hydrogen and helium ions. <i>Physical Review B</i> , 2011 , 83,	3.3	33
87	Room-temperature ferromagnetism via unpaired dopant electrons and p π coupling in carbon-doped In ₂ O ₃ : Experiment and theory. <i>Physical Review B</i> , 2012 , 86,	3.3	31
86	The role of surface chemical reactivity in the stability of electronic nanodevices based on two-dimensional materials Beyond graphene and topological insulators. <i>FlatChem</i> , 2017 , 1, 60-64	5.1	29
85	The atomic and electronic structure of nitrogen- and boron-doped phosphorene. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 27210-6	3.6	29
84	Sn-loss effect in a Sn-implanted a-SiO ₂ host-matrix after thermal annealing: A combined XPS, PL, and DFT study. <i>Applied Surface Science</i> , 2016 , 367, 320-326	6.7	29
83	Electronic structure of magnetic molecules V15: LSDA+U calculations, x-ray emissions, and photoelectron spectra. <i>Physical Review B</i> , 2003 , 67,	3.3	29
82	Toward the Effective Exploitation of Topological Phases of Matter in Catalysis: Chemical Reactions at the Surfaces of NbAs and TaAs Weyl Semimetals. <i>Advanced Functional Materials</i> , 2018 , 28, 1800511	15.6	26
81	Modeling of epitaxial graphene functionalization. <i>Nanotechnology</i> , 2011 , 22, 055708	3.4	26
80	Formation of a Quasi-Free-Standing Single Layer of Graphene and Hexagonal Boron Nitride on Pt(111) by a Single Molecular Precursor. <i>Advanced Functional Materials</i> , 2016 , 26, 1120-1126	15.6	26
79	Atomic and electronic structures of stable linear carbon chains on Ag-nanoparticles. <i>Carbon</i> , 2018 , 128, 296-301	10.4	25
78	Effect of ligand substitution on the exchange interactions in {Mn(12)}-type single-molecule magnets. <i>Inorganic Chemistry</i> , 2010 , 49, 10902-6	5.1	24
77	Ligand-controlled magnetic interactions in Mn(4) clusters. <i>Inorganic Chemistry</i> , 2009 , 48, 11903-8	5.1	24
76	Study of the Structural Characteristics of 3d Metals Cr, Mn, Fe, Co, Ni, and Cu Implanted in ZnO and TiO ₂ Experiment and Theory. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 28143-28151	3.8	23
75	Self-Assembled SnO/SnSe Heterostructures: A Suitable Platform for Ultrasensitive NO and H Sensing. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 34362-34369	9.5	23

74	XPS and DFT study of pulsed Bi-implantation of bulk and thin-films of ZnO. The role of oxygen imperfections. <i>Applied Surface Science</i> , 2016 , 387, 1093-1099	6.7	23
73	Hydrogen dissociation catalyzed by carbon-coated nickel nanoparticles: experiment and theory. <i>ChemPhysChem</i> , 2013 , 14, 381-5	3.2	22
72	Unveiling the Origin of the High Catalytic Activity of Ultrathin 1T/2H MoSe Nanosheets for the Hydrogen Evolution Reaction: A Combined Experimental and Theoretical Study. <i>ChemSusChem</i> , 2019 , 12, 5015-5022	8.3	21
71	The MRO-accompanied modes of Re-implantation into SiO ₂ -host matrix: XPS and DFT based scenarios. <i>Journal of Alloys and Compounds</i> , 2017 , 728, 759-766	5.7	21
70	Metal-Organic Frameworks for the Adsorptive Removal of Gaseous Aliphatic Ketones. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 10317-10331	9.5	18
69	XPS and DFT study of Sn incorporation into ZnO and TiO ₂ host matrices by pulsed ion implantation. <i>Physica Status Solidi (B): Basic Research</i> , 2015 , 252, 1890-1896	1.3	18
68	Transition-Metal Dichalcogenide NiTe ₂ : An Ambient-Stable Material for Catalysis and Nanoelectronics. <i>Advanced Functional Materials</i> , 2020 , 30, 2000915	15.6	17
67	Modulation of Volmer step for efficient alkaline water splitting implemented by titanium oxide promoting surface reconstruction of cobalt carbonate hydroxide. <i>Nano Energy</i> , 2021 , 82, 105732	17.1	17
66	Utilization of metal-organic frameworks for the adsorptive removal of an aliphatic aldehyde mixture in the gas phase. <i>Nanoscale</i> , 2020 , 12, 8330-8343	7.7	16
65	Octahedral conversion of α -SiO ₂ host matrix by pulsed ion implantation. <i>Physica Status Solidi (B): Basic Research</i> , 2015 , 252, 2185-2190	1.3	16
64	Modification of titanium and titanium dioxide surfaces by ion implantation: Combined XPS and DFT study. <i>Physica Status Solidi (B): Basic Research</i> , 2015 , 252, 748-754	1.3	16
63	PdTe ₂ Transition-Metal Dichalcogenide: Chemical Reactivity, Thermal Stability, and Device Implementation. <i>Advanced Functional Materials</i> , 2020 , 30, 1906556	15.6	16
62	Structural phase transitions in VSe: energetics, electronic structure and magnetism. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 22647-22653	3.6	15
61	XPS spectra as a tool for studying photochemical and thermal degradation in APbX ₃ hybrid halide perovskites. <i>Nano Energy</i> , 2021 , 79, 105421	17.1	15
60	Application of Zr-Cluster-Based MOFs for the Adsorptive Removal of Aliphatic Aldehydes (C to C) from an Industrial Solvent. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 44270-44281	9.5	14
59	A new triboelectric nanogenerator with excellent electric breakdown self-healing performance. <i>Nano Energy</i> , 2021 , 85, 105990	17.1	14
58	Unusually strong lateral interaction in the CO overlayer in phosphorene-based systems. <i>Nano Research</i> , 2016 , 9, 2598-2605	10	14
57	First-principles modeling of the interactions of iron impurities with graphene and graphite. <i>Physica Status Solidi (B): Basic Research</i> , 2011 , 248, 1347-1351	1.3	13

56	Charge Redistribution Mechanisms in SnSe Surfaces Exposed to Oxidative and Humid Environments and Their Related Influence on Chemical Sensing. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 9003-9011	6.4	13
55	Molecular dynamics simulation insight into the temperature dependence and healing mechanism of an intrinsic self-healing polyurethane elastomer. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 17620-17631	3.6	13
54	Bi-doped silica glass: A combined XPS DFT study of electronic structure and pleomorphic imperfections. <i>Journal of Alloys and Compounds</i> , 2020 , 829, 154459	5.7	12
53	Structural defects and electronic structure of N-ion implanted TiO ₂ : Bulk versus thin film. <i>Applied Surface Science</i> , 2015 , 355, 984-988	6.7	10
52	Cellulose Hydrogels by Reversible Ion-Exchange as Flexible Pressure Sensors. <i>Advanced Materials Technologies</i> , 2020 , 5, 2000358	6.8	10
51	Understanding Mechanism of Adsorption in the Decolorization of Aqueous Methyl Violet (6B) Solution by Okra Polysaccharides: Experiment and Theory. <i>ACS Omega</i> , 2019 , 4, 17880-17889	3.9	10
50	Atomic, electronic and magnetic structure of graphene/iron and nickel interfaces: theory and experiment. <i>RSC Advances</i> , 2015 , 5, 9173-9179	3.7	9
49	Development of Theoretical Descriptors for Cytotoxicity Evaluation of Metallic Nanoparticles. <i>Chemical Research in Toxicology</i> , 2017 , 30, 1549-1555	4	9
48	Unveiling the origin of room-temperature ferromagnetism in monolayer VSe: the role of extrinsic effects. <i>Nanoscale</i> , 2020 , 12, 20875-20882	7.7	9
47	Amine-functionalized microporous covalent organic polymers for adsorptive removal of a gaseous aliphatic aldehyde mixture. <i>Environmental Science: Nano</i> , 2020 , 7, 3447-3468	7.1	9
46	Influence of Ion Migration from ITO and SiO ₂ Substrates on Photo and Thermal Stability of CH ₃ NH ₃ SnI ₃ Hybrid Perovskite. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 14928-14934	3.8	8
45	Synthesis and Magnetic Properties of Mn ¹² -Based Single Molecular Magnets with Benzene and Pentafluorobenzene Carboxylate Ligands. <i>Journal of Superconductivity and Novel Magnetism</i> , 2011 , 24, 855-859	1.5	8
44	Efficient hydrogen evolution reaction with platinum stannide PtSn ₄ via surface oxidation. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 2349-2355	13	8
43	Absence of a stable atomic structure in fluorinated graphene. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 13287-93	3.6	8
42	Chemical reactions on surfaces for applications in catalysis, gas sensing, adsorption-assisted desalination and Li-ion batteries: opportunities and challenges for surface science. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 7541-7552	3.6	8
41	H-bond/ionic coordination switching for fabrication of highly oriented cellulose hydrogels. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 5533-5541	13	8
40	Noncovalent bonding of copper atoms to the nitrogen-containing sites of hydrogenated diamond surfaces. <i>Mendeleev Communications</i> , 2019 , 29, 452-454	1.9	7
39	Under-cover stabilization and reactivity of a dense carbon monoxide layer on Pt(111). <i>Chemical Science</i> , 2019 , 10, 1857-1865	9.4	7

38	Local atomic configurations, energy structure, and optical properties of implantation defects in Gd-doped silica glass: An XPS, PL, and DFT study. <i>Journal of Alloys and Compounds</i> , 2019 , 796, 77-85	5.7	7
37	Bulk vs. Surface Structure of 3d Metal Impurities in Topological Insulator BiTe. <i>Scientific Reports</i> , 2017 , 7, 5758	4.9	7
36	Terahertz Photodetection with Type-II Dirac Fermions in Transition-Metal Ditellurides and Their Heterostructures. <i>Physica Status Solidi - Rapid Research Letters</i> , 2021 , 15, 2100212	2.5	7
35	Formation of FeTe Antiferromagnetic Dimers in Doped TiO ₂ :Fe Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 1494-1505	3.8	6
34	First-principle studies of optical properties of Be Zn ₁ -O ternary mixed crystal. <i>Optik</i> , 2019 , 178, 691-697	2.5	6
33	Atomic and electronic structure of graphene oxide/Cu interface. <i>Thin Solid Films</i> , 2018 , 665, 99-108	2.2	6
32	Bulk In ₂ O ₃ crystals grown by chemical vapour transport: a combination of XPS and DFT studies. <i>Journal of Materials Science: Materials in Electronics</i> , 2019 , 30, 18753-18758	2.1	5
31	Effect of doping and annealing on the electronic structure and magnetic properties of nanoscale Co and Zn co-doped SnO ₂ : An experimental study and first-principles modeling. <i>Journal of Alloys and Compounds</i> , 2019 , 799, 433-441	5.7	5
30	Surface Instability and Chemical Reactivity of ZrSiS and ZrSiSe Nodal-Line Semimetals. <i>Advanced Functional Materials</i> , 2019 , 29, 1900438	15.6	5
29	Unconventional magnetism of non-uniform distribution of Co in TiO ₂ nanoparticles. <i>Journal of Alloys and Compounds</i> , 2020 , 826, 154194	5.7	5
28	Enhancing Reverse Saturable Absorption in SnS Nanosheets by Plasma Treatment. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 4211-4219	9.5	5
27	Thermal Effects and Halide Mixing of Hybrid Perovskites: MD and XPS Studies. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 135-140	2.8	4
26	Hybrid Surface Passivation for Retrieving Charge Collection Efficiency of Colloidal Quantum Dot Photovoltaics. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 43576-43585	9.5	4
25	Interaction of graphene oxide with barium titanate in composite: XPS and DFT studies. <i>Journal of Alloys and Compounds</i> , 2020 , 840, 155747	5.7	3
24	Chemical instability of free-standing boron monolayers and properties of oxidized borophene sheets. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020 , 120, 114082	3	3
23	Catalytic activity of PtSn ₄ : Insights from surface-science spectroscopies. <i>Applied Surface Science</i> , 2020 , 514, 145925	6.7	3
22	Computational calculation identified optimal binding sites in nano-sized magnetic-cored dendrimer. <i>Chemosphere</i> , 2018 , 210, 287-295	8.4	3
21	Enhanced clustering tendency of Cu-impurities with a number of oxygen vacancies in heavy carbon-loaded TiO ₂ - the bulk and surface morphologies. <i>Solid State Sciences</i> , 2017 , 71, 130-138	3.4	3

20	Efficient Electrochemical Water Splitting with PdSn ₄ Dirac Nodal Arc Semimetal. <i>ACS Catalysis</i> , 2021 , 11, 7311-7318	13.1	3
19	Interaction of VSe ₂ with Ambient Gases: Stability and Chemical Reactivity. <i>Physica Status Solidi - Rapid Research Letters</i> , 2020 , 14, 1900332	2.5	3
18	Effect of long-term storage on the electronic structure of semiconducting silicon wafers implanted by rhenium ions. <i>Journal of Materials Science</i> , 2021 , 56, 2103-2112	4.3	3
17	Kitkaite NiTeSe, an Ambient-Stable Layered Dirac Semimetal with Low-Energy Type-II Fermions with Application Capabilities in Spintronics and Optoelectronics. <i>Advanced Functional Materials</i> , 2021 , 31, 2106101	15.6	3
16	Quality assessment of GaN epitaxial films: Acidification scenarios based on XPS-and-DFT combined study. <i>Applied Surface Science</i> , 2021 , 563, 150308	6.7	3
15	Sequestration of carbon monoxide at room temperature at vacancy sites of graphene. <i>Chemical Communications</i> , 2019 , 55, 8607-8610	5.8	2
14	Electronic structure and structural defects in 3d-metal doped In ₂ O ₃ . <i>Journal of Materials Science: Materials in Electronics</i> , 2019 , 30, 14091-14098	2.1	1
13	Reactive adsorption and catalytic oxidation of gaseous formaldehyde at room temperature by a synergistic copper-magnesium bimetal oxide biochar composite. <i>Chemical Engineering Journal</i> , 2021 , 433, 133497	14.7	1
12	X-ray photoelectron spectra and electronic structure of Mo doped V ₂ O ₅ . <i>Thin Solid Films</i> , 2020 , 713, 138360	2.2	1
11	Unveiling the Mechanisms Ruling the Efficient Hydrogen Evolution Reaction with Mitrofanovite PtTe. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 8627-8636	6.4	1
10	First-Principles Modeling of Atomic Structure and Chemical and Optical Properties of EC ₃ N ₄ . <i>Journal of Carbon Research</i> , 2019 , 5, 58	3.3	0
9	Engineering ferromagnetic lines in graphene by local oxidation and hydrogenation using nanoscale lithography. <i>Journal Physics D: Applied Physics</i> , 2021 , 54, 074002	3	0
8	Unveiling the Atomic and Electronic Structure of Stacked-Cup Carbon Nanofibers. <i>Nanoscale Research Letters</i> , 2021 , 16, 153	5	0
7	Mitrofanovite PtTe: A Topological Metal with Termination-Dependent Surface Band Structure and Strong Spin Polarization. <i>ACS Nano</i> , 2021 , 15, 14786-14793	16.7	0
6	Low-temperature oxidative removal of gaseous formaldehyde by an eggshell waste supported silver-manganese dioxide bimetallic catalyst with ultralow noble metal content.. <i>Journal of Hazardous Materials</i> , 2022 , 434, 128857	12.8	0
5	Structure and Magnetic Properties of Superoxide Radical Anion Complexes with Low Binding Energy at the Graphene Edges. <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2020 , 46, 738-745	1.6	0
4	Uncommon clustering in dilute TiBe alloys. <i>JPhys Materials</i> , 2020 , 3, 025007	4.2	0
3	Fabrication of Conjugated Porous Polymer Catalysts for Oxygen Reduction Reactions: A Bottom-Up Approach. <i>Catalysts</i> , 2020 , 10, 1224	4	0

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| 2 | Long range interactions and related carbon-carbon bond reconstruction between interior and surface defects in nanodiamonds. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 14592-14600 | 3.6 |
| 1 | Effect of vacancy defects on electronic structure and ferromagnetism in pristine In ₂ O ₃ nanostructures: An experimental study and first-principles modeling. <i>Materials Research Bulletin</i> , 2022 , 152, 111853 | 5.1 |