

Oleg V Yazyev

List of Publications by Year in descending order

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160
papers

17,395
citations

34016

52
h-index

13338

130
g-index

165
all docs

165
docs citations

165
times ranked

19765
citing authors

#	ARTICLE	IF	CITATIONS
1	2D transition metal dichalcogenides. Nature Reviews Materials, 2017, 2, .	23.3	3,689
2	Defect-induced magnetism in graphene. Physical Review B, 2007, 75, .	1.1	1,268
3	Emergence of magnetism in graphene materials and nanostructures. Reports on Progress in Physics, 2010, 73, 056501.	8.1	1,026
4	Electronic transport in polycrystalline graphene. Nature Materials, 2010, 9, 806-809.	13.3	839
5	Topological defects in graphene: Dislocations and grain boundaries. Physical Review B, 2010, 81, .	1.1	659
6	Magnetic Correlations at Graphene Edges: Basis for Novel Spintronics Devices. Physical Review Letters, 2008, 100, 047209.	2.9	646
7	Spatially resolving edge states of chiral graphene nanoribbons. Nature Physics, 2011, 7, 616-620.	6.5	628
8	Spin Polarization and Transport of Surface States in the Topological Insulators Bi_2Se_3 Bi_2Te_3 First Principles. Physical Review Letters, 2010, 105, 266806.	2.9	424
9	Magnetism in Disordered Graphene and Irradiated Graphite. Physical Review Letters, 2008, 101, 037203.	2.9	408
10	Polycrystalline graphene and other two-dimensional materials. Nature Nanotechnology, 2014, 9, 755-767.	15.6	408
11	Correlated states in twisted double bilayer graphene. Nature Physics, 2020, 16, 520-525.	6.5	374
12	Z2Pack: Numerical implementation of hybrid Wannier centers for identifying topological materials. Physical Review B, 2017, 95, .	1.1	322
13	Observation of Weyl nodes and Fermi arcs in tantalum phosphide. Nature Communications, 2016, 7, 11006.	5.8	264
14	Topological Frustration in Graphene Nanoflakes: Magnetic Order and Spin Logic Devices. Physical Review Letters, 2009, 102, 157201.	2.9	237
15	Atomic Scale Microstructure and Properties of Se-Deficient Two-Dimensional MoSe ₂ . ACS Nano, 2015, 9, 3274-3283.	7.3	213
16	Identifying substitutional oxygen as a prolific point defect in monolayer transition metal dichalcogenides. Nature Communications, 2019, 10, 3382.	5.8	196
17	Effect of Metal Elements in Catalytic Growth of Carbon Nanotubes. Physical Review Letters, 2008, 100, 156102.	2.9	189
18	A Guide to the Design of Electronic Properties of Graphene Nanoribbons. Accounts of Chemical Research, 2013, 46, 2319-2328.	7.6	187

#	ARTICLE	IF	CITATIONS
19	MoS ₂ and semiconductors in the flatland. Materials Today, 2015, 18, 20-30.	8.3	179
20	Robust Type-II Weyl Semimetal Phase in Transition Metal Diphosphides X		

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37	Hyperfine Interactions in Graphene and Related Carbon Nanostructures. Nano Letters, 2008, 8, 1011-1015.	4.5	99
38	A novel quasi-one-dimensional topological insulator in bismuth iodide \hat{I}^2 -Bi ₄ I ₄ . Nature Materials, 2016, 15, 154-158.	13.3	90
39	Non-Abelian reciprocal braiding of Weyl points and its manifestation in ZrTe. Nature Physics, 2020, 16, 1137-1143.	6.5	87
40	Metal adatoms on graphene and hexagonal boron nitride: Towards rational design of self-assembly templates. Physical Review B, 2010, 82, .	1.1	84
41	Defects in bilayer silica and graphene: common trends in diverse hexagonal two-dimensional systems. Scientific Reports, 2013, 3, 3482.	1.6	80
42	Comment on Graphene Nanoflakes with Large Spin: Broken-Symmetry States. Nano Letters, 2008, 8, 766-766.	4.5	76
43	Infrared- and Raman-Spectroscopy Measurements of a Transition in the Crystal Structure and a Closing of the Energy Gap of BiTeI under Pressure. Physical Review Letters, 2014, 112, 047402.	2.9	71
44	Early stages of radiation damage in graphite and carbon nanostructures: A first-principles molecular dynamics study. Physical Review B, 2007, 75, .	1.1	68
45	Template Nanowires for Spintronics Applications: Nanomagnet Microwave Resonators Functioning in Zero Applied Magnetic Field. Nano Letters, 2008, 8, 3683-3687.	4.5	67
46	Highly Oriented Atomically Thin Ambipolar MoSe ₂ Grown by Molecular Beam Epitaxy. ACS Nano, 2017, 11, 6355-6361.	7.3	64
47	Probing magnetism in atomically thin semiconducting PtSe ₂ . Nature Communications, 2020, 11, 4806.	5.8	63
48	Probing the Out-of-Plane Distortion of Single Point Defects in Atomically Thin Hexagonal Boron Nitride at the Picometer Scale. Physical Review Letters, 2011, 106, 126102.	2.9	62
49	Magnetoresistance from Fermi surface topology. Physical Review B, 2019, 99, .	1.1	60
50	Muons Probe Strong Hydrogen Interactions with Defective Graphene. Nano Letters, 2011, 11, 4919-4922.	4.5	58
51	Artificial Neural Network Approach to the Analytic Continuation Problem. Physical Review Letters, 2020, 124, 056401.	2.9	58
52	Spin- and valley-polarized transport across line defects in monolayer MoS ₂ . Physical Review B, 2016, 93, .	1.1	58
53	Subangstrom Edge Relaxations Probed by Electron Microscopy in Hexagonal Boron Nitride. Physical Review Letters, 2012, 109, 205502.	2.9	52
54	Origin of Fine Structure in Si ₂ p Photoelectron Spectra at Silicon Surfaces and Interfaces. Physical Review Letters, 2006, 96, 157601.	2.9	51

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55	Quantum Chemical Investigation of Hyperfine Coupling Constants on First Coordination Sphere Water Molecule of Gadolinium(III) Aqua Complexes. Journal of Physical Chemistry A, 2005, 109, 10997-11005.	1.1	49
56	Gadolinium (III) ion in liquid water: Structure, dynamics, and magnetic interactions from first principles. Journal of Chemical Physics, 2007, 127, 084506.	1.2	49
57	Point defects in the MoS_2 monolayer phases of single-layer MoS_2 . Physical Review Letters, 2019, 122, 176402.	1.1	48
58	Radial Spin Texture of the Weyl Fermions in Chiral Tellurium. Physical Review Letters, 2020, 125, 216402.	2.9	47
59	Grain Boundaries in Graphene on SiC(0001 $\bar{1}$...) Substrate. Nano Letters, 2014, 14, 6382-6386.	4.5	46
60	Electromechanical oscillations in bilayer graphene. Nature Communications, 2015, 6, 8582.	5.8	44
61	Observation of a nodal chain with Dirac surface states in TiB_2 . Physical Review B, 2018, 97, .	1.1	44
62	Topological Aspects of Charge-Carrier Transmission across Grain Boundaries in Graphene. Nano Letters, 2014, 14, 250-254.	4.5	43
63	Observation of Weyl Nodes in Robust Type-II Weyl Semimetal WP_2 . Physical Review Letters, 2019, 122, 176402.	2.9	42
64	Extremely large magnetoresistance in the topologically trivial semimetal TaAs . Physical Review B, 2018, 97, .	1.1	41
65	Core spin-polarization correction in pseudopotential-based electronic structure calculations. Physical Review B, 2005, 71, .	1.1	39
66	Magnetic Excitations and Electronic Interactions in Sr_2VO_4 . Physical Review Letters, 2016, 117, 237203.	2.9	36
67	A Spin-Charge density wave phase, Mottness, and ferromagnetism in monolayer TaSe_2 . Physical Review B, 2018, 98, .	1.1	35
68	Topological phase transitions driven by strain in monolayer tellurium. Physical Review B, 2018, 98, .	1.1	34
69	Strong out-of-plane magnetic anisotropy of Fe adatoms on Bi_2Te_3 . Physical Review B, 2014, 89, .	1.1	32
70	Magnetic exchange interactions in monolayer CrI_3 from many-body wavefunction calculations. 2D Materials, 2020, 7, 035005.	2.0	32
71	Electronic instability in a Zero-Gap Semiconductor: The Charge-Density Wave in TaSe_4I . Physical Review Letters, 2013, 110, 236401.	1.1	31
72	Manipulating Topological Domain Boundaries in the Single-Layer Quantum Spin Hall Insulator WSe_2 . Nano Letters, 2019, 19, 5634-5639.	4.5	30

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73	Crystal field, ligand field, and interorbital effects in two-dimensional transition metal dichalcogenides across the periodic table. 2D Materials, 2019, 6, 025015.	2.0	30
74	Electronic Transport in Graphene with Aggregated Hydrogen Adatoms. Physical Review Letters, 2014, 113, 246601.	2.9	29
75	Momentum and photon energy dependence of the circular dichroic photoemission in the bulk Rashba semiconductors BiTeX (X = Sb, As). Physical Review Letters, 2014, 113, 246601.	2.9	29
76	Kinetic studies on the first dihydrogen aquacomplex, $[\text{Ru}(\text{H}_2)(\text{H}_2\text{O})_5]^{2+}$: Formation under H_2 pressure and catalytic H/D isotope exchange in water. Inorganica Chimica Acta, 2006, 359, 1795-1806.	1.2	28
77	Nuclear Spin Relaxation Parameters of MRI Contrast Agents – Insight from Quantum Mechanical Calculations. European Journal of Inorganic Chemistry, 2008, 2008, 201-211.	1.0	28
78	Inducing Magnetic Phase Transitions in Monolayer CrI_3 via Lattice Deformations. Journal of Physical Chemistry C, 2020, 124, 7585-7590.	1.5	28
79	Distinct Evolutions of Weyl Fermion Quasiparticles and Fermi Arcs with Bulk Band Topology in Weyl Semimetals. Physical Review Letters, 2017, 118, 106406.	2.9	27
80	Efficient algorithm for band connectivity resolution. Physical Review B, 2002, 65, .	1.1	26
81	Localized electronic states at grain boundaries on the surface of graphene and graphite. 2D Materials, 2016, 3, 031005.	2.0	26
82	Enhanced ultrafast relaxation rate in the Weyl semimetal phase of MoTe_2 measured by time- and angle-resolved photoelectron spectroscopy. Physical Review B, 2017, 96, .	1.1	26
83	Coexistence of tunable Weyl points and topological nodal lines in ternary transition-metal telluride TaIrTe_4 . Physical Review B, 2018, 97, .	1.1	26
84	Multiplet features and magnetic properties of Fe on $\text{Cu}(111)$: From single atoms to small clusters. Physical Review B, 2015, 91, .	1.1	25
85	Pressure effect and superconductivity in the CaAgP topological phase. Physical Review B, 2018, 97, .	1.1	25
86	Trivial topological phase of CaAgP and the topological nodal-line transition in CaAgP . Physical Review B, 2018, 97, .	1.1	25
87	^{17}O nuclear quadrupole coupling constants of water bound to a metal ion: A gadolinium(III) case study. Journal of Chemical Physics, 2006, 125, 054503.	1.2	23
88	Excitonic effects in two-dimensional TiSe_2 from hybrid density functional theory. Physical Review B, 2018, 98, .	1.1	23
89	Highly anisotropic interlayer magnetoresistance in ZrSiS nodal-line Dirac semimetal. Physical Review B, 2019, 100, .	1.1	23
90	Exchange Interactions Mediated by Nonmagnetic Cations in Double Perovskites. Physical Review Letters, 2020, 124, 077202.	2.9	23

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91	Edge Disorder in Bottom-Up Zigzag Graphene Nanoribbons: Implications for Magnetism and Quantum Electronic Transport. Journal of Physical Chemistry Letters, 2021, 12, 4692-4696.	2.1	22
92	Isotropic Knight shift of metallic carbon nanotubes. Physical Review B, 2005, 72, .	1.1	21
93	Atomic and electronic structure of a Rashba δ surface at the BiTeI surface. Physical Review B, 2014, 89, .		
94	Polycrystalline graphene: Atomic structure, energetics and transport properties. Solid State Communications, 2012, 152, 1431-1436.	0.9	18
95	Engineering the topological surface states in the δ surface with width="0.16em"		

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109	Structural Phase Transition and Bandgap Control through Mechanical Deformation in Layered Semiconductors $1T\bar{d}ZrX_2$ ($X = S, Se$)., 2020, 2, 1115-1120.		15
110	Electronic transport across quantum dots in graphene nanoribbons: Toward built-in gap-tunable metal-semiconductor-metal heterojunctions. Physical Review B, 2020, 102, .	1.1	15
111	Observation of a singular Weyl point surrounded by charged nodal walls in PtGa. Nature Communications, 2021, 12, 3994.	5.8	15
112	Hyperfine interactions in aqueous solution of Cr^{3+} : an ab initio molecular dynamics study. Theoretical Chemistry Accounts, 2006, 115, 190-195.	0.5	14
113	Coherent generation of symmetry-forbidden phonons by light-induced electron-phonon interactions in magnetite. Physical Review B, 2017, 96, .	1.1	14
114	Linear and quadratic magnetoresistance in the semimetal Pb_2Si . Physical Review B, 2020, 102, .	1.1	14
115	Temperature dependence of quantum oscillations from non-parabolic dispersions. Nature Communications, 2021, 12, 6213.	5.8	14
116	Single-layer $1T\bar{d}MoS_2$ under electron irradiation from ab initio molecular dynamics. 2D Materials, 2018, 5, 025022.	2.0	13
117	Ab initio theory of magnetism in two-dimensional Cr_2Te . Physical Review B, 2022, 105, .		
118	An upside-down magnet. Nature Physics, 2019, 15, 424-425.	6.5	12
119	Light induced electron spin resonance properties of van der Waals CrX_3 ($X = Cl, I$) crystals. Applied Physics Letters, 2020, 117, .	1.5	12
120	Dirac fermions at high-index surfaces of bismuth chalcogenide topological insulator nanostructures. Scientific Reports, 2016, 6, 20220.	1.6	11
121	square lattice antiferromagnetism in the orbitally quenched insulator Mo_4OPO_4 . Physical Review B, 2017, 96, .	1.1	10
122	Robustness of the quantum spin Hall insulator phase in monolayer $1T\bar{d}$ transition metal dichalcogenides. Journal of Electron Spectroscopy and Related Phenomena, 2017, 219, 72-76.	0.8	9
123	Landau levels of the Euler class topology. Physical Review Research, 2022, 4, .	1.3	9
124	$BiTeCl$ and $BiTeBr$: A comparative high-pressure optical study. Physical Review B, 2017, 95, .	1.1	8
125	Unified picture of lattice instabilities in metallic transition metal dichalcogenides. Physical Review B, 2019, 100, .	1.1	8
126	Transport signatures of temperature-induced chemical potential shift and Lifshitz transition in layered type-II Weyl semimetal $TaIrTe_4$. 2D Materials, 2021, 8, 015020.	2.0	8

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127	Unidirectional Kondo scattering in layered NbS ₂ . Npj 2D Materials and Applications, 2021, 5, .	3.9	8
128	Multiple mobile excitons manifested as sidebands in quasi-one-dimensional metallic TaSe ₃ . Nature Materials, 2022, 21, 423-429.	13.3	8
129	Controlling the Quantum Spin Hall Edge States in Two-Dimensional Transition Metal Dichalcogenides. Journal of Physical Chemistry Letters, 2020, 11, 6964-6969.	2.1	7
130	Hidden bulk and surface effects in the spin polarization of the nodal-line semimetal ZrSiTe. Communications Physics, 2021, 4, .	2.0	7
131	Nature of native atomic defects in $ZrTe_5$ and their impact on the low-energy electronic structure. Physical Review Materials, 2020, 4, .		
132	Magnetism induced by single-atom defects in nanographites. Journal of Physics: Conference Series, 2007, 61, 1294-1298.	0.3	6
133	Theory of Magnetism in Graphene. Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems, 2012, 2, 71-103.	0.6	6
134	Structural and electronic properties of the Bi/Au(110) $\sqrt{3}\times\sqrt{3}$ surface. Physical Review B, 2013, 88, .	1.1	6
135	Controlling edge states in the Kane-Mele model via edge chirality. Physica Status Solidi - Rapid Research Letters, 2013, 7, 151-153.	1.2	6
136	Lattice-matched heterojunctions between topological and normal insulators: A first-principles study. Physical Review B, 2017, 95, .	1.1	6
137	Even-odd conductance effect in graphene nanoribbons induced by edge functionalization with aromatic molecules: basis for novel chemosensors. European Physical Journal Plus, 2020, 135, 1.	1.2	6
138	One-dimensional structural irregularities in graphene: chiral edges and grain boundaries. Journal of Physics: Conference Series, 2011, 302, 012016.	0.3	5
139	Crystal Field Effect and Electric Field Screening in Multilayer Graphene with and without Twist. Nano Letters, 2021, 21, 4636-4642.	4.5	5
140	SrPt ₈ As: a layered incommensurately modulated metal with saturated resistivity. IUCr, 2018, 5, 470-477.	1.0	5
141	Phase transition of layer-stacked borophene under pressure. Physical Review B, 2022, 105, .	1.1	5
142	A finite temperature linear tetrahedron method for electronic structure calculations of periodic systems. Journal of Chemical Physics, 2004, 121, 2466.	1.2	4
143	Interplay between spin-orbit coupling and crystal-field effect in topological insulators. Journal of Physics Condensed Matter, 2015, 27, 285801.	0.7	4
144	Electronic properties of one-dimensional nanostructures of the Bi_2X_3 topological insulator. Physical Review B, 2018, 97, .		

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145	Topological Fermi-arc surface resonances in bcc iron. Physical Review B, 2020, 102, .	1.1	4
146	Giant Chern number of a Weyl nodal surface without upper limit. Physical Review B, 2022, 105, .	1.1	4
147	Intercalant-mediated Kitaev exchange in OAg_3O_6 . Physical Review Research, 2022, 4, .	1.3	4
148	Muons probe magnetism and hydrogen interaction in graphene. Physica Scripta, 2013, 88, 068508.	1.2	3
149	Theory of Magnetism in Graphitic Materials. Springer Series in Materials Science, 2016, , 1-24.	0.4	3
150	Hydrogen Bonding of Ammonia with (H ₂ O)-Si(001) Revealed by Experimental and Ab Initio Photoelectron Spectroscopy. Journal of Physical Chemistry A, 2020, 124, 5378-5388.	1.1	3
151	Magnetization Signature of Topological Surface States in a Non-Centrosymmetric Superconductor. Advanced Materials, 2021, 33, e2103257.	11.1	3
152	Extremely large magnetoresistance in the "ordinary" metal ReO_3 . Physical Review B, 2021, 104, .	1.1	3
153	Origin of large magnetoresistance in the topological nonsymmorphic semimetal TaSe ₃ . Physical Review B, 2021, 104, .	1.1	2
154	Core-Level Photoelectron Spectroscopy Probing Local Strain at Silicon Surfaces and Interfaces. AIP Conference Proceedings, 2007, , .	0.3	1
155	Modeling Disordered and Nanostructured Graphene. , 2020, , 53-72.		1
156	Charge ordering in Ir dimers in the ground state of Ba ₅ AlIr ₂ O ₁₁ . Physical Review B, 2022, 105, .	1.1	1
157	Metal catalyst in CVD growth of carbon nanotubes: role of chemical composition. , 2010, , .		0
158	Possibility of an unconventional spin state of Ir ⁴⁺ in Ba ₂ Ir ₉ O ₄₃ single crystal. Physical Review B, 2016, 94, .	1.1	0
159	Modeling Disordered and Nanostructured Graphene. , 2018, , 1-20.		0
160	Electronic properties of incommensurately modulated novel and complex materials. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e96-e96.	0.0	0