

Oleg V Yazyev

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

145
papers

13,183
citations

48
h-index

114
g-index

165
ext. papers

15,416
ext. citations

7.6
avg, IF

7.23
L-index

#	Paper	IF	Citations
145	Unidirectional Kondo scattering in layered NbS ₂ . <i>Npj 2D Materials and Applications</i> , 2021 , 5,	8.8	1
144	Temperature dependence of quantum oscillations from non-parabolic dispersions. <i>Nature Communications</i> , 2021 , 12, 6213	17.4	1
143	Transport signatures of temperature-induced chemical potential shift and Lifshitz transition in layered type-II Weyl semimetal TaIrTe ₄ . <i>2D Materials</i> , 2021 , 8, 015020	5.9	4
142	Quantum electronic transport across bit defects in graphene nanoribbons. <i>2D Materials</i> , 2021 , 8, 035025	5.9	5
141	Crystal Field Effect and Electric Field Screening in Multilayer Graphene with and without Twist. <i>Nano Letters</i> , 2021 , 21, 4636-4642	11.5	3
140	Edge Disorder in Bottom-Up Zigzag Graphene Nanoribbons: Implications for Magnetism and Quantum Electronic Transport. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 4692-4696	6.4	4
139	Observation of a singular Weyl point surrounded by charged nodal walls in PtGa. <i>Nature Communications</i> , 2021 , 12, 3994	17.4	1
138	Landau Levels as a Probe for Band Topology in Graphene Moiré Superlattices. <i>Physical Review Letters</i> , 2021 , 126, 056401	7.4	4
137	Hidden bulk and surface effects in the spin polarization of the nodal-line semimetal ZrSiTe. <i>Communications Physics</i> , 2021 , 4,	5.4	3
136	Magnetization Signature of Topological Surface States in a Non-Symmorphic Superconductor. <i>Advanced Materials</i> , 2021 , 33, e2103257	24	
135	Linear and quadratic magnetoresistance in the semimetal SiP ₂ . <i>Physical Review B</i> , 2020 , 102,	3.3	4
134	Electronic transport across quantum dots in graphene nanoribbons: Toward built-in gap-tunable metal-semiconductor-metal heterojunctions. <i>Physical Review B</i> , 2020 , 102,	3.3	7
133	Magnetic exchange interactions in monolayer CrI ₃ from many-body wavefunction calculations. <i>2D Materials</i> , 2020 , 7, 035005	5.9	17
132	Hydrogen Bonding of Ammonia with (H ₂ O)-Si(001) Revealed by Experimental and Ab Initio Photoelectron Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 5378-5388	2.8	1
131	Inducing Magnetic Phase Transitions in Monolayer CrI ₃ via Lattice Deformations. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 7585-7590	3.8	13
130	Correlated states in twisted double bilayer graphene. <i>Nature Physics</i> , 2020 , 16, 520-525	16.2	194
129	Artificial Neural Network Approach to the Analytic Continuation Problem. <i>Physical Review Letters</i> , 2020 , 124, 056401	7.4	17

128	Moiré Flat Bands in Twisted Double Bilayer Graphene. <i>Nano Letters</i> , 2020 , 20, 2410-2415	11.5	54
127	Exchange Interactions Mediated by Nonmagnetic Cations in Double Perovskites. <i>Physical Review Letters</i> , 2020 , 124, 077202	7.4	6
126	Modeling Disordered and Nanostructured Graphene 2020 , 53-72		1
125	Large magnetoresistance and nonzero Berry phase in the nodal-line semimetal MoO ₂ . <i>Physical Review B</i> , 2020 , 102,	3.3	6
124	Probing magnetism in atomically thin semiconducting PtSe. <i>Nature Communications</i> , 2020 , 11, 4806	17.4	28
123	Topological Fermi-arc surface resonances in bcc iron. <i>Physical Review B</i> , 2020 , 102,	3.3	1
122	Non-Abelian reciprocal braiding of Weyl points and its manifestation in ZrTe. <i>Nature Physics</i> , 2020 , 16, 1137-1143	16.2	20
121	Radial Spin Texture of the Weyl Fermions in Chiral Tellurium. <i>Physical Review Letters</i> , 2020 , 125, 216402	7.4	8
120	Controlling the Quantum Spin Hall Edge States in Two-Dimensional Transition Metal Dichalcogenides. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 6964-6969	6.4	0
119	Structural Phase Transition and Bandgap Control through Mechanical Deformation in Layered Semiconductors 1T _x R ₂ X ₂ (X = S, Se) 2020 , 2, 1115-1120		1
118	Light induced electron spin resonance properties of van der Waals CrX ₃ (X = Cl, I) crystals. <i>Applied Physics Letters</i> , 2020 , 117, 082406	3.4	4
117	Even-odd conductance effect in graphene nanoribbons induced by edge functionalization with aromatic molecules: basis for novel chemosensors. <i>European Physical Journal Plus</i> , 2020 , 135, 1	3.1	3
116	The 2021 quantum materials roadmap. <i>JPhys Materials</i> , 2020 , 3, 042006	4.2	48
115	Highly anisotropic interlayer magnetoresistance in ZrSiS nodal-line Dirac semimetal. <i>Physical Review B</i> , 2019 , 100,	3.3	8
114	Crystal field, ligand field, and interorbital effects in two-dimensional transition metal dichalcogenides across the periodic table. <i>2D Materials</i> , 2019 , 6, 025015	5.9	15
113	Magnetoresistance from Fermi surface topology. <i>Physical Review B</i> , 2019 , 99,	3.3	26
112	Defect induced, layer-modulated magnetism in ultrathin metallic PtSe. <i>Nature Nanotechnology</i> , 2019 , 14, 674-678	28.7	106
111	Observation of Weyl Nodes in Robust Type-II Weyl Semimetal WP ₂ . <i>Physical Review Letters</i> , 2019 , 122, 176402	7.4	21

110	Manipulating Topological Domain Boundaries in the Single-Layer Quantum Spin Hall Insulator 1T'-WSe. <i>Nano Letters</i> , 2019 , 19, 5634-5639	11.5	18
109	Identifying substitutional oxygen as a prolific point defect in monolayer transition metal dichalcogenides. <i>Nature Communications</i> , 2019 , 10, 3382	17.4	117
108	Unified picture of lattice instabilities in metallic transition metal dichalcogenides. <i>Physical Review B</i> , 2019 , 100,	3.3	3
107	Single-layer 1 T'-MoS ₂ under electron irradiation from ab initio molecular dynamics. <i>2D Materials</i> , 2018 , 5, 025022	5.9	8
106	Trivial topological phase of CaAgP and the topological nodal-line transition in CaAg(P _{1-x} As _x). <i>Physical Review B</i> , 2018 , 97,	3.3	14
105	Electronic properties of one-dimensional nanostructures of the Bi ₂ Se ₃ topological insulator. <i>Physical Review B</i> , 2018 , 97,	3.3	4
104	Reinvestigating the surface and bulk electronic properties of Cd ₃ As ₂ . <i>Physical Review B</i> , 2018 , 97,	3.3	13
103	Structural and electronic transformation in low-angle twisted bilayer graphene. <i>2D Materials</i> , 2018 , 5, 015019	5.9	84
102	Charge density wave phase, Mottness, and ferromagnetism in monolayer 1T-NbSe ₂ . <i>Physical Review B</i> , 2018 , 98,	3.3	21
101	Observation of a nodal chain with Dirac surface states in TiB ₂ . <i>Physical Review B</i> , 2018 , 97,	3.3	26
100	Observation of topologically protected states at crystalline phase boundaries in single-layer WSe. <i>Nature Communications</i> , 2018 , 9, 3401	17.4	68
99	MgTa ₂ N ₃ : A reference Dirac semimetal. <i>Physical Review B</i> , 2018 , 98,	3.3	12
98	Extremely large magnetoresistance in the topologically trivial semimetal WP ₂ . <i>Physical Review B</i> , 2018 , 97,	3.3	25
97	Coexistence of tunable Weyl points and topological nodal lines in ternary transition-metal telluride TaIrTe ₄ . <i>Physical Review B</i> , 2018 , 97,	3.3	18
96	SrPtAs: a layered incommensurately modulated metal with saturated resistivity. <i>IUCrJ</i> , 2018 , 5, 470-477	4.7	2
95	Excitonic effects in two-dimensional TiSe ₂ from hybrid density functional theory. <i>Physical Review B</i> , 2018 , 98,	3.3	16
94	Modeling Disordered and Nanostructured Graphene 2018 , 1-20		
93	Electronic Properties of Transferable Atomically Thin MoSe ₂ /h-BN Heterostructures Grown on Rh(111). <i>ACS Nano</i> , 2018 , 12, 11161-11168	16.7	14

92	Topological phase transitions driven by strain in monolayer tellurium. <i>Physical Review B</i> , 2018 , 98,	3.3	22
91	BiTeCl and BiTeBr: A comparative high-pressure optical study. <i>Physical Review B</i> , 2017 , 95,	3.3	7
90	Distinct Evolutions of Weyl Fermion Quasiparticles and Fermi Arcs with Bulk Band Topology in Weyl Semimetals. <i>Physical Review Letters</i> , 2017 , 118, 106406	7.4	23
89	Two-Orbital Kondo Screening in a Self-Assembled Metal-Organic Complex. <i>ACS Nano</i> , 2017 , 11, 2675-2681.	6.7	12
88	Highly Oriented Atomically Thin Ambipolar MoSe Grown by Molecular Beam Epitaxy. <i>ACS Nano</i> , 2017 , 11, 6355-6361	16.7	48
87	2D transition metal dichalcogenides. <i>Nature Reviews Materials</i> , 2017 , 2,	7.3	22.13
86	Persistence of a surface state arc in the topologically trivial phase of MoTe ₂ . <i>Physical Review B</i> , 2017 , 95,	3.3	16
85	Z2Pack: Numerical implementation of hybrid Wannier centers for identifying topological materials. <i>Physical Review B</i> , 2017 , 95,	3.3	23.0
84	Lattice-matched heterojunctions between topological and normal insulators: A first-principles study. <i>Physical Review B</i> , 2017 , 95,	3.3	5
83	Coherent generation of symmetry-forbidden phonons by light-induced electron-phonon interactions in magnetite. <i>Physical Review B</i> , 2017 , 96,	3.3	10
82	J1J ₂ square lattice antiferromagnetism in the orbitally quenched insulator MoOPO ₄ . <i>Physical Review B</i> , 2017 , 96,	3.3	6
81	Pressure effect and superconductivity in the Bi ₄ I ₄ topological insulator. <i>Physical Review B</i> , 2017 , 95,	3.3	22
80	Point defects in the 1T' and 2H phases of single-layer MoS ₂ : A comparative first-principles study. <i>Physical Review B</i> , 2017 , 96,	3.3	39
79	Robustness of the quantum spin Hall insulator phase in monolayer 1T' transition metal dichalcogenides. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2017 , 219, 72-76	1.7	7
78	Temperature dependent non-monotonic bands shift in ZrTe ₅ . <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2017 , 219, 9-15	1.7	13
77	Enhanced ultrafast relaxation rate in the Weyl semimetal phase of MoTe ₂ measured by time- and angle-resolved photoelectron spectroscopy. <i>Physical Review B</i> , 2017 , 96,	3.3	20
76	Optically switched magnetism in photovoltaic perovskite CH ₃ NH(Mn:Pb)I ₃ . <i>Nature Communications</i> , 2016 , 7, 13406	17.4	85
75	Observation of Weyl nodes and Fermi arcs in tantalum phosphide. <i>Nature Communications</i> , 2016 , 7, 11006.	7.4	22.4

74	Spin- and valley-polarized transport across line defects in monolayer MoS ₂ . <i>Physical Review B</i> , 2016 , 93,	3.3	37
73	Theory of Magnetism in Graphitic Materials. <i>Springer Series in Materials Science</i> , 2016 , 1-24	0.9	1
72	Disorder engineering and conductivity dome in ReS ₂ with electrolyte gating. <i>Nature Communications</i> , 2016 , 7, 12391	17.4	89
71	A novel quasi-one-dimensional topological insulator in bismuth iodide BiI ₃ . <i>Nature Materials</i> , 2016 , 15, 154-8	27	64
70	Evidence for a Strong Topological Insulator Phase in ZrTe ₅ . <i>Physical Review Letters</i> , 2016 , 117, 237601	7.4	89
69	Magnetic Excitations and Electronic Interactions in Sr ₂ CuTeO ₆ : A Spin-1/2 Square Lattice Heisenberg Antiferromagnet. <i>Physical Review Letters</i> , 2016 , 117, 237203	7.4	22
68	Dirac fermions at high-index surfaces of bismuth chalcogenide topological insulator nanostructures. <i>Scientific Reports</i> , 2016 , 6, 20220	4.9	10
67	Localized electronic states at grain boundaries on the surface of graphene and graphite. <i>2D Materials</i> , 2016 , 3, 031005	5.9	26
66	Robust Type-II Weyl Semimetal Phase in Transition Metal Diphosphides XP ₂ (X=Mo, W). <i>Physical Review Letters</i> , 2016 , 117, 066402	7.4	131
65	MoS ₂ and semiconductors in the flatland. <i>Materials Today</i> , 2015 , 18, 20-30	21.8	126
64	Atomic scale microstructure and properties of Se-deficient two-dimensional MoSe ₂ . <i>ACS Nano</i> , 2015 , 9, 3274-83	16.7	176
63	Interplay between spin-orbit coupling and crystal-field effect in topological insulators. <i>Journal of Physics Condensed Matter</i> , 2015 , 27, 285801	1.8	3
62	Density Functional Theory Calculations of Topological Insulators 2015 , 131-160		0
61	Electromechanical oscillations in bilayer graphene. <i>Nature Communications</i> , 2015 , 6, 8582	17.4	34
60	Engineering the topological surface states in the (Sb ₂) _m (Bi ₂) _{3-m} Te ₃ (m=0-3) superlattice series. <i>Physical Review B</i> , 2015 , 91,	3.3	17
59	Multiplet features and magnetic properties of Fe on Cu(111): From single atoms to small clusters. <i>Physical Review B</i> , 2015 , 91,	3.3	20
58	Bulk and surface band structure of the new family of semiconductors BiTeX (X=I, Br, Cl). <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2015 , 201, 115-120	1.7	15
57	Infrared- and Raman-spectroscopy measurements of a transition in the crystal structure and a closing of the energy gap of BiTeI under pressure. <i>Physical Review Letters</i> , 2014 , 112, 047402	7.4	61

56	Topological aspects of charge-carrier transmission across grain boundaries in graphene. <i>Nano Letters</i> , 2014 , 14, 250-4	11.5	41
55	Grain boundaries in graphene on SiC(0001) substrate. <i>Nano Letters</i> , 2014 , 14, 6382-6	11.5	40
54	Polycrystalline graphene and other two-dimensional materials. <i>Nature Nanotechnology</i> , 2014 , 9, 755-67	28.7	338
53	Strong out-of-plane magnetic anisotropy of Fe adatoms on Bi ₂ Te ₃ . <i>Physical Review B</i> , 2014 , 89,	3.3	26
52	Momentum and photon energy dependence of the circular dichroic photoemission in the bulk Rashba semiconductors BiTeX (X=I, Br, Cl). <i>Physical Review B</i> , 2014 , 89,	3.3	21
51	Controlled growth of a line defect in graphene and implications for gate-tunable valley filtering. <i>Physical Review B</i> , 2014 , 89,	3.3	96
50	Electronic transport in graphene with aggregated hydrogen adatoms. <i>Physical Review Letters</i> , 2014 , 113, 246601	7.4	28
49	Atomic and electronic structure of a Rashba p \bar{n} junction at the BiTeI surface. <i>Physical Review B</i> , 2014 , 89,	3.3	19
48	Magnetic moment and anisotropy of individual Co atoms on graphene. <i>Physical Review Letters</i> , 2013 , 111, 236801	7.4	97
47	Defects in bilayer silica and graphene: common trends in diverse hexagonal two-dimensional systems. <i>Scientific Reports</i> , 2013 , 3, 3482	4.9	71
46	Engineering quantum spin Hall effect in graphene nanoribbons via edge functionalization. <i>Physical Review B</i> , 2013 , 87,	3.3	14
45	A guide to the design of electronic properties of graphene nanoribbons. <i>Accounts of Chemical Research</i> , 2013 , 46, 2319-28	24.3	138
44	Experimentally engineering the edge termination of graphene nanoribbons. <i>ACS Nano</i> , 2013 , 7, 198-202	16.7	132
43	Muons probe magnetism and hydrogen interaction in graphene. <i>Physica Scripta</i> , 2013 , 88, 068508	2.6	3
42	Electronic instability in a zero-gap semiconductor: the charge-density wave in (TaSe ₄) ₂ I. <i>Physical Review Letters</i> , 2013 , 110, 236401	7.4	17
41	Structural and electronic properties of the Bi/Au(110) $\sqrt{3}\sqrt{3}$ surface. <i>Physical Review B</i> , 2013 , 88,	3.3	3
40	Controlling edge states in the Kane-Mele model via edge chirality. <i>Physica Status Solidi - Rapid Research Letters</i> , 2013 , 7, 151-153	2.5	6
39	Polycrystalline graphene: Atomic structure, energetics and transport properties. <i>Solid State Communications</i> , 2012 , 152, 1431-1436	1.6	16

38	Giant ambipolar Rashba effect in the semiconductor BiTeI. <i>Physical Review Letters</i> , 2012 , 109, 096803	7.4	139
37	Theory of Magnetism in Graphene. <i>Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems</i> , 2012 , 2, 71-103		6
36	Quasiparticle effects in the bulk and surface-state bands of Bi ₂ Se ₃ and Bi ₂ Te ₃ topological insulators. <i>Physical Review B</i> , 2012 , 85,	3.3	101
35	Subangstrom edge relaxations probed by electron microscopy in hexagonal boron nitride. <i>Physical Review Letters</i> , 2012 , 109, 205502	7.4	44
34	Muons probe strong hydrogen interactions with defective graphene. <i>Nano Letters</i> , 2011 , 11, 4919-22	11.5	54
33	One-dimensional structural irregularities in graphene: chiral edges and grain boundaries. <i>Journal of Physics: Conference Series</i> , 2011 , 302, 012016	0.3	3
32	Spatially resolving edge states of chiral graphene nanoribbons. <i>Nature Physics</i> , 2011 , 7, 616-620	16.2	557
31	Theory of magnetic edge states in chiral graphene nanoribbons. <i>Physical Review B</i> , 2011 , 84,	3.3	96
30	Probing the out-of-plane distortion of single point defects in atomically thin hexagonal boron nitride at the picometer scale. <i>Physical Review Letters</i> , 2011 , 106, 126102	7.4	57
29	Electronic transport in polycrystalline graphene. <i>Nature Materials</i> , 2010 , 9, 806-9	27	756
28	Metal adatoms on graphene and hexagonal boron nitride: Towards rational design of self-assembly templates. <i>Physical Review B</i> , 2010 , 82,	3.3	78
27	Spin polarization and transport of surface states in the topological insulators Bi ₂ Se ₃ and Bi ₂ Te ₃ from first principles. <i>Physical Review Letters</i> , 2010 , 105, 266806	7.4	381
26	Emergence of magnetism in graphene materials and nanostructures. <i>Reports on Progress in Physics</i> , 2010 , 73, 056501	14.4	865
25	Topological defects in graphene: Dislocations and grain boundaries. <i>Physical Review B</i> , 2010 , 81,	3.3	571
24	Magnetoresistive junctions based on epitaxial graphene and hexagonal boron nitride. <i>Physical Review B</i> , 2009 , 80,	3.3	98
23	Scaling properties of flexible membranes from atomistic simulations: Application to graphene. <i>Physical Review B</i> , 2009 , 80,	3.3	126
22	Topological frustration in graphene nanoflakes: magnetic order and spin logic devices. <i>Physical Review Letters</i> , 2009 , 102, 157201	7.4	209
21	Effect of metal elements in catalytic growth of carbon nanotubes. <i>Physical Review Letters</i> , 2008 , 100, 156102	7.4	176

20	Hyperfine interactions in graphene and related carbon nanostructures. <i>Nano Letters</i> , 2008 , 8, 1011-5	11.5	87
19	Comment on graphene nanoflakes with large spin: broken-symmetry states. <i>Nano Letters</i> , 2008 , 8, 766	11.5	70
18	Template nanowires for spintronics applications: nanomagnet microwave resonators functioning in zero applied magnetic field. <i>Nano Letters</i> , 2008 , 8, 3683-7	11.5	59
17	Carbon diffusion in CVD growth of carbon nanotubes on metal nanoparticles. <i>Physica Status Solidi (B): Basic Research</i> , 2008 , 245, 2185-2188	1.3	14
16	Nuclear Spin Relaxation Parameters of MRI Contrast Agents – Insight from Quantum Mechanical Calculations. <i>European Journal of Inorganic Chemistry</i> , 2008 , 2008, 201-211	2.3	25
15	Magnetic correlations at graphene edges: basis for novel spintronics devices. <i>Physical Review Letters</i> , 2008 , 100, 047209	7.4	566
14	Magnetism in disordered graphene and irradiated graphite. <i>Physical Review Letters</i> , 2008 , 101, 037203	7.4	371
13	Defect-induced magnetism in graphene. <i>Physical Review B</i> , 2007 , 75,	3.3	1107
12	Gadolinium (III) ion in liquid water: structure, dynamics, and magnetic interactions from first principles. <i>Journal of Chemical Physics</i> , 2007 , 127, 084506	3.9	43
11	Magnetism induced by single-atom defects in nanographites. <i>Journal of Physics: Conference Series</i> , 2007 , 61, 1294-1298	0.3	6
10	Early stages of radiation damage in graphite and carbon nanostructures: A first-principles molecular dynamics study. <i>Physical Review B</i> , 2007 , 75,	3.3	66
9	Hyperfine interactions in aqueous solution of Cr ³⁺ : an ab initio molecular dynamics study. <i>Theoretical Chemistry Accounts</i> , 2006 , 115, 190-195	1.9	13
8	Origin of fine structure in si photoelectron spectra at silicon surfaces and interfaces. <i>Physical Review Letters</i> , 2006 , 96, 157601	7.4	50
7	¹⁷ O nuclear quadrupole coupling constants of water bound to a metal ion: a gadolinium(III) case study. <i>Journal of Chemical Physics</i> , 2006 , 125, 054503	3.9	20
6	Kinetic studies on the first dihydrogen aquacomplex, [Ru(H ₂)(H ₂ O) ₅] ²⁺ : Formation under H ₂ pressure and catalytic H/D isotope exchange in water. <i>Inorganica Chimica Acta</i> , 2006 , 359, 1795-1806	2.7	27
5	Core spin-polarization correction in pseudopotential-based electronic structure calculations. <i>Physical Review B</i> , 2005 , 71,	3.3	30
4	Quantum chemical investigation of hyperfine coupling constants on first coordination sphere water molecule of gadolinium(III) aqua complexes. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 10997-1005	2.8	43
3	Isotropic Knight shift of metallic carbon nanotubes. <i>Physical Review B</i> , 2005 , 72,	3.3	21

- 2 A finite temperature linear tetrahedron method for electronic structure calculations of periodic systems. *Journal of Chemical Physics*, **2004**, 121, 2466-70 3.9 4
- 1 Efficient algorithm for band connectivity resolution. *Physical Review B*, **2002**, 65, 3.3 26