# Oleg V Yazyev

#### List of Publications by Citations

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13,183 48 145 114 h-index g-index citations papers 165 15,416 7.6 7.23 L-index avg, IF ext. citations ext. papers

#	Paper	IF	Citations
145	2D transition metal dichalcogenides. <i>Nature Reviews Materials</i> , <b>2017</b> , 2,	73.3	2213
144	Defect-induced magnetism in graphene. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	1107
143	Emergence of magnetism in graphene materials and nanostructures. <i>Reports on Progress in Physics</i> , <b>2010</b> , 73, 056501	14.4	865
142	Electronic transport in polycrystalline graphene. <i>Nature Materials</i> , <b>2010</b> , 9, 806-9	27	756
141	Topological defects in graphene: Dislocations and grain boundaries. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	57 <sup>1</sup>
140	Magnetic correlations at graphene edges: basis for novel spintronics devices. <i>Physical Review Letters</i> , <b>2008</b> , 100, 047209	7.4	566
139	Spatially resolving edge states of chiral graphene nanoribbons. <i>Nature Physics</i> , <b>2011</b> , 7, 616-620	16.2	557
138	Spin polarization and transport of surface states in the topological insulators Bi2Se3 and Bi2Te3 from first principles. <i>Physical Review Letters</i> , <b>2010</b> , 105, 266806	7.4	381
137	Magnetism in disordered graphene and irradiated graphite. <i>Physical Review Letters</i> , <b>2008</b> , 101, 037203	7.4	371
136	Polycrystalline graphene and other two-dimensional materials. <i>Nature Nanotechnology</i> , <b>2014</b> , 9, 755-67	28.7	338
135	Z2Pack: Numerical implementation of hybrid Wannier centers for identifying topological materials. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	230
134	Observation of Weyl nodes and Fermi arcs in tantalum phosphide. <i>Nature Communications</i> , <b>2016</b> , 7, 110	0 <del>.6</del> 7.4	224
133	Topological frustration in graphene nanoflakes: magnetic order and spin logic devices. <i>Physical Review Letters</i> , <b>2009</b> , 102, 157201	7.4	209
132	Correlated states in twisted double bilayer graphene. <i>Nature Physics</i> , <b>2020</b> , 16, 520-525	16.2	194
131	Atomic scale microstructure and properties of Se-deficient two-dimensional MoSe2. <i>ACS Nano</i> , <b>2015</b> , 9, 3274-83	16.7	176
130	Effect of metal elements in catalytic growth of carbon nanotubes. <i>Physical Review Letters</i> , <b>2008</b> , 100, 156102	7.4	176
129	Giant ambipolar Rashba effect in the semiconductor BiTel. <i>Physical Review Letters</i> , <b>2012</b> , 109, 096803	7.4	139

### (2010-2013)

128	A guide to the design of electronic properties of graphene nanoribbons. <i>Accounts of Chemical Research</i> , <b>2013</b> , 46, 2319-28	24.3	138
127	Experimentally engineering the edge termination of graphene nanoribbons. <i>ACS Nano</i> , <b>2013</b> , 7, 198-20	216.7	132
126	Robust Type-II Weyl Semimetal Phase in Transition Metal Diphosphides XP_{2} (X=Mo, W). <i>Physical Review Letters</i> , <b>2016</b> , 117, 066402	7.4	131
125	MoS 2 and semiconductors in the flatland. <i>Materials Today</i> , <b>2015</b> , 18, 20-30	21.8	126
124	Scaling properties of flexible membranes from atomistic simulations: Application to graphene. <i>Physical Review B</i> , <b>2009</b> , 80,	3.3	126
123	Identifying substitutional oxygen as a prolific point defect in monolayer transition metal dichalcogenides. <i>Nature Communications</i> , <b>2019</b> , 10, 3382	17.4	117
122	Defect induced, layer-modulated magnetism in ultrathin metallic PtSe. <i>Nature Nanotechnology</i> , <b>2019</b> , 14, 674-678	28.7	106
121	Quasiparticle effects in the bulk and surface-state bands of Bi2Se3 and Bi2Te3 topological insulators. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	101
120	Magnetoresistive junctions based on epitaxial graphene and hexagonal boron nitride. <i>Physical Review B</i> , <b>2009</b> , 80,	3.3	98
119	Magnetic moment and anisotropy of individual Co atoms on graphene. <i>Physical Review Letters</i> , <b>2013</b> , 111, 236801	7.4	97
118	Controlled growth of a line defect in graphene and implications for gate-tunable valley filtering. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	96
117	Theory of magnetic edge states in chiral graphene nanoribbons. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	96
116	Disorder engineering and conductivity dome in ReS2 with electrolyte gating. <i>Nature Communications</i> , <b>2016</b> , 7, 12391	17.4	89
115	Evidence for a Strong Topological Insulator Phase in ZrTe_{5}. <i>Physical Review Letters</i> , <b>2016</b> , 117, 23760	)1 <sub>7.4</sub>	89
114	Hyperfine interactions in graphene and related carbon nanostructures. <i>Nano Letters</i> , <b>2008</b> , 8, 1011-5	11.5	87
113	Optically switched magnetism in photovoltaic perovskite CHNH(Mn:Pb)I. <i>Nature Communications</i> , <b>2016</b> , 7, 13406	17.4	85
112	Structural and electronic transformation in low-angle twisted bilayer graphene. 2D Materials, 2018, 5, 015019	5.9	84
111	Metal adatoms on graphene and hexagonal boron nitride: Towards rational design of self-assembly templates. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	78

110	Defects in bilayer silica and graphene: common trends in diverse hexagonal two-dimensional systems. <i>Scientific Reports</i> , <b>2013</b> , 3, 3482	4.9	71
109	Comment on graphene nanoflakes with large spin: broken-symmetry states. <i>Nano Letters</i> , <b>2008</b> , 8, 766	11.5	70
108	Observation of topologically protected states at crystalline phase boundaries in single-layer WSe. <i>Nature Communications</i> , <b>2018</b> , 9, 3401	17.4	68
107	Early stages of radiation damage in graphite and carbon nanostructures: A first-principles molecular dynamics study. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	66
106	A novel quasi-one-dimensional topological insulator in bismuth iodide EBi4I4. <i>Nature Materials</i> , <b>2016</b> , 15, 154-8	27	64
105	Infrared- and Raman-spectroscopy measurements of a transition in the crystal structure and a closing of the energy gap of BiTel under pressure. <i>Physical Review Letters</i> , <b>2014</b> , 112, 047402	7.4	61
104	Template nanowires for spintronics applications: nanomagnet microwave resonators functioning in zero applied magnetic field. <i>Nano Letters</i> , <b>2008</b> , 8, 3683-7	11.5	59
103	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> , <b>2011</b> , 106, 126102	7.4	57
102	Moir[Flat Bands in Twisted Double Bilayer Graphene. Nano Letters, 2020, 20, 2410-2415	11.5	54
101	Muons probe strong hydrogen interactions with defective graphene. <i>Nano Letters</i> , <b>2011</b> , 11, 4919-22	11.5	54
100	Origin of fine structure in si photoelectron spectra at silicon surfaces and interfaces. <i>Physical Review Letters</i> , <b>2006</b> , 96, 157601	7.4	50
99	Highly Oriented Atomically Thin Ambipolar MoSe Grown by Molecular Beam Epitaxy. <i>ACS Nano</i> , <b>2017</b> , 11, 6355-6361	16.7	48
98	The 2021 quantum materials roadmap. <i>JPhys Materials</i> , <b>2020</b> , 3, 042006	4.2	48
97	Subangstrom edge relaxations probed by electron microscopy in hexagonal boron nitride. <i>Physical Review Letters</i> , <b>2012</b> , 109, 205502	7.4	44
96	Gadolinium (III) ion in liquid water: structure, dynamics, and magnetic interactions from first principles. <i>Journal of Chemical Physics</i> , <b>2007</b> , 127, 084506	3.9	43
95	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> , <b>2005</b> , 109, 10997-1005	2.8	43
94	Topological aspects of charge-carrier transmission across grain boundaries in graphene. <i>Nano Letters</i> , <b>2014</b> , 14, 250-4	11.5	41
93	Grain boundaries in graphene on SiC(0001) substrate. <i>Nano Letters</i> , <b>2014</b> , 14, 6382-6	11.5	40

## (2018-2017)

92	Point defects in the 1T? and 2H phases of single-layer MoS2: A comparative first-principles study. <i>Physical Review B</i> , <b>2017</b> , 96,	3.3	39	
91	Spin- and valley-polarized transport across line defects in monolayer MoS2. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	37	
90	Electromechanical oscillations in bilayer graphene. Nature Communications, 2015, 6, 8582	17.4	34	
89	Core spin-polarization correction in pseudopotential-based electronic structure calculations. <i>Physical Review B</i> , <b>2005</b> , 71,	3.3	30	
88	Electronic transport in graphene with aggregated hydrogen adatoms. <i>Physical Review Letters</i> , <b>2014</b> , 113, 246601	7.4	28	
87	Probing magnetism in atomically thin semiconducting PtSe. <i>Nature Communications</i> , <b>2020</b> , 11, 4806	17.4	28	
86	Kinetic studies on the first dihydrogen aquacomplex, [Ru(H2)(H2O)5]2+: Formation under H2 pressure and catalytic H/D isotope exchange in water. <i>Inorganica Chimica Acta</i> , <b>2006</b> , 359, 1795-1806	2.7	27	
85	Magnetoresistance from Fermi surface topology. <i>Physical Review B</i> , <b>2019</b> , 99,	3.3	26	
84	Observation of a nodal chain with Dirac surface states in TiB2. Physical Review B, 2018, 97,	3.3	26	
83	Strong out-of-plane magnetic anisotropy of Fe adatoms on Bi2Te3. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	26	
82	Efficient algorithm for band connectivity resolution. <i>Physical Review B</i> , <b>2002</b> , 65,	3.3	26	
81	Localized electronic states at grain boundaries on the surface of graphene and graphite. <i>2D Materials</i> , <b>2016</b> , 3, 031005	5.9	26	
80	Extremely large magnetoresistance in the topologically trivial semimetal WP2. <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	25	
79	Nuclear Spin Relaxation Parameters of MRI Contrast Agents Insight from Quantum Mechanical Calculations. <i>European Journal of Inorganic Chemistry</i> , <b>2008</b> , 2008, 201-211	2.3	25	
78	Distinct Evolutions of Weyl Fermion Quasiparticles and Fermi Arcs with Bulk Band Topology in Weyl Semimetals. <i>Physical Review Letters</i> , <b>2017</b> , 118, 106406	7.4	23	
77	Pressure effect and superconductivity in the <b>B</b> i4l4 topological insulator. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	22	
76	Magnetic Excitations and Electronic Interactions in Sr_{2}CuTeO_{6}: A Spin-1/2 Square Lattice Heisenberg Antiferromagnet. <i>Physical Review Letters</i> , <b>2016</b> , 117, 237203	7·4	22	
75	Topological phase transitions driven by strain in monolayer tellurium. <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	22	

74	Observation of Weyl Nodes in Robust Type-II Weyl Semimetal WP_{2}. <i>Physical Review Letters</i> , <b>2019</b> , 122, 176402	7.4	21
73	Charge density wave phase, Mottness, and ferromagnetism in monolayer 1TNbSe2. <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	21
72	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> , <b>2014</b> , 89,	3.3	21
71	Isotropic Knight shift of metallic carbon nanotubes. <i>Physical Review B</i> , <b>2005</b> , 72,	3.3	21
70	Enhanced ultrafast relaxation rate in the Weyl semimetal phase of MoTe2 measured by time- and angle-resolved photoelectron spectroscopy. <i>Physical Review B</i> , <b>2017</b> , 96,	3.3	20
69	Multiplet features and magnetic properties of Fe on Cu(111): From single atoms to small clusters. <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	20
68	17O nuclear quadrupole coupling constants of water bound to a metal ion: a gadolinium(III) case study. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 054503	3.9	20
67	Non-Abelian reciprocal braiding of Weyl points and its manifestation in ZrTe. <i>Nature Physics</i> , <b>2020</b> , 16, 1137-1143	16.2	20
66	Atomic and electronic structure of a Rashba pli junction at the BiTeI surface. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	19
65	Coexistence of tunable Weyl points and topological nodal lines in ternary transition-metal telluride TaIrTe4. <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	18
64	Manipulating Topological Domain Boundaries in the Single-Layer Quantum Spin Hall Insulator 1T'-WSe. <i>Nano Letters</i> , <b>2019</b> , 19, 5634-5639	11.5	18
63	Magnetic exchange interactions in monolayer CrI3 from many-body wavefunction calculations. <i>2D Materials</i> , <b>2020</b> , 7, 035005	5.9	17
62	Artificial Neural Network Approach to the Analytic Continuation Problem. <i>Physical Review Letters</i> , <b>2020</b> , 124, 056401	7.4	17
61	Engineering the topological surface states in the (Sb2)mBb2Te3(m=0B) superlattice series. <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	17
60	Electronic instability in a zero-gap semiconductor: the charge-density wave in (TaSe4)21. <i>Physical Review Letters</i> , <b>2013</b> , 110, 236401	7.4	17
59	Persistence of a surface state arc in the topologically trivial phase of MoTe2. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	16
58	Polycrystalline graphene: Atomic structure, energetics and transport properties. <i>Solid State Communications</i> , <b>2012</b> , 152, 1431-1436	1.6	16
57	Excitonic effects in two-dimensional TiSe2 from hybrid density functional theory. <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	16

56	Crystal field, ligand field, and interorbital effects in two-dimensional transition metal dichalcogenides across the periodic table. 2D Materials, 2019, 6, 025015	5.9	15	
55	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> , <b>2015</b> , 201, 115-120	1.7	15	
54	Trivial topological phase of CaAgP and the topological nodal-line transition in CaAg(P1🏼Asx). <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	14	
53	Engineering quantum spin Hall effect in graphene nanoribbons via edge functionalization. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	14	
52	Carbon diffusion in CVD growth of carbon nanotubes on metal nanoparticles. <i>Physica Status Solidi</i> (B): Basic Research, <b>2008</b> , 245, 2185-2188	1.3	14	
51	Electronic Properties of Transferable Atomically Thin MoSe/h-BN Heterostructures Grown on Rh(111). <i>ACS Nano</i> , <b>2018</b> , 12, 11161-11168	16.7	14	
50	Inducing Magnetic Phase Transitions in Monolayer CrI3via Lattice Deformations. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 7585-7590	3.8	13	
49	Reinvestigating the surface and bulk electronic properties of Cd3As2. <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	13	
48	Temperature dependent non-monotonic bands shift in ZrTe5. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , <b>2017</b> , 219, 9-15	1.7	13	
47	Hyperfine interactions in aqueous solution of Cr3+: an ab initio molecular dynamics study. <i>Theoretical Chemistry Accounts</i> , <b>2006</b> , 115, 190-195	1.9	13	
46	Two-Orbital Kondo Screening in a Self-Assembled Metal-Organic Complex. ACS Nano, 2017, 11, 2675-26	<b>81</b> 6.7	12	
45	MgTa2N3: A reference Dirac semimetal. <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	12	
44	Coherent generation of symmetry-forbidden phonons by light-induced electron-phonon interactions in magnetite. <i>Physical Review B</i> , <b>2017</b> , 96,	3.3	10	
43	Dirac fermions at high-index surfaces of bismuth chalcogenide topological insulator nanostructures. <i>Scientific Reports</i> , <b>2016</b> , 6, 20220	4.9	10	
42	Highly anisotropic interlayer magnetoresitance in ZrSiS nodal-line Dirac semimetal. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	8	
41	Single-layer 1 T ?-MoS 2 under electron irradiation from ab initio molecular dynamics. <i>2D Materials</i> , <b>2018</b> , 5, 025022	5.9	8	
40	Radial Spin Texture of the Weyl Fermions in Chiral Tellurium. <i>Physical Review Letters</i> , <b>2020</b> , 125, 216402	₹7.4	8	
39	BiTeCl and BiTeBr: A comparative high-pressure optical study. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	7	

38	Electronic transport across quantum dots in graphene nanoribbons: Toward built-in gap-tunable metal-semiconductor-metal heterojunctions. <i>Physical Review B</i> , <b>2020</b> , 102,	3.3	7
37	Robustness of the quantum spin Hall insulator phase in monolayer 1T? transition metal dichalcogenides. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , <b>2017</b> , 219, 72-76	1.7	7
36	Exchange Interactions Mediated by Nonmagnetic Cations in Double Perovskites. <i>Physical Review Letters</i> , <b>2020</b> , 124, 077202	7.4	6
35	J1🏿 square lattice antiferromagnetism in the orbitally quenched insulator MoOPO4. <i>Physical Review B</i> , <b>2017</b> , 96,	3.3	6
34	Theory of Magnetism in Graphene. <i>Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems</i> , <b>2012</b> , 2, 71-103		6
33	Controlling edge states in the KaneMele model via edge chirality. <i>Physica Status Solidi - Rapid Research Letters</i> , <b>2013</b> , 7, 151-153	2.5	6
32	Magnetism induced by single-atom defects in nanographites. <i>Journal of Physics: Conference Series</i> , <b>2007</b> , 61, 1294-1298	0.3	6
31	Large magnetoresistance and nonzero Berry phase in the nodal-line semimetal MoO2. <i>Physical Review B</i> , <b>2020</b> , 102,	3.3	6
30	Lattice-matched heterojunctions between topological and normal insulators: A first-principles study. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	5
29	Quantum electronic transport across Biteldefects in graphene nanoribbons. 2D Materials, 2021, 8, 035	5 <b>025</b> 9	5
28	Linear and quadratic magnetoresistance in the semimetal SiP2. Physical Review B, 2020, 102,	3.3	4
27	Electronic properties of one-dimensional nanostructures of the Bi2Se3 topological insulator. <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	4
26	A finite temperature linear tetrahedron method for electronic structure calculations of periodic systems. <i>Journal of Chemical Physics</i> , <b>2004</b> , 121, 2466-70	3.9	4
25	Transport signatures of temperature-induced chemical potential shift and Lifshitz transition in layered type-II Weyl semimetal TaIrTe4. 2D Materials, <b>2021</b> , 8, 015020	5.9	4
24	Light induced electron spin resonance properties of van der Waals CrX3 (X = Cl, I) crystals. <i>Applied Physics Letters</i> , <b>2020</b> , 117, 082406	3.4	4
23	Edge Disorder in Bottom-Up Zigzag Graphene Nanoribbons: Implications for Magnetism and Quantum Electronic Transport. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 4692-4696	6.4	4
22	Landau Levels as a Probe for Band Topology in Graphene Moir Superlattices. <i>Physical Review Letters</i> , <b>2021</b> , 126, 056401	7.4	4
21	Interplay between spin-orbit coupling and crystal-field effect in topological insulators. <i>Journal of Physics Condensed Matter</i> , <b>2015</b> , 27, 285801	1.8	3

## (2020-2013)

20	Muons probe magnetism and hydrogen interaction in graphene. <i>Physica Scripta</i> , <b>2013</b> , 88, 068508	2.6	3
19	Structural and electronic properties of the Bi/Au(110) III surface. Physical Review B, 2013, 88,	3.3	3
18	One-dimensional structural irregularities in graphene: chiral edges and grain boundaries. <i>Journal of Physics: Conference Series</i> , <b>2011</b> , 302, 012016	0.3	3
17	EvenBdd conductance effect in graphene nanoribbons induced by edge functionalization with aromatic molecules: basis for novel chemosensors. <i>European Physical Journal Plus</i> , <b>2020</b> , 135, 1	3.1	3
16	Crystal Field Effect and Electric Field Screening in Multilayer Graphene with and without Twist. <i>Nano Letters</i> , <b>2021</b> , 21, 4636-4642	11.5	3
15	Unified picture of lattice instabilities in metallic transition metal dichalcogenides. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	3
14	Hidden bulk and surface effects in the spin polarization of the nodal-line semimetal ZrSiTe. <i>Communications Physics</i> , <b>2021</b> , 4,	5.4	3
13	SrPt As: a layered incommensurately modulated metal with saturated resistivity. <i>IUCrJ</i> , <b>2018</b> , 5, 470-47	74.7	2
12	Hydrogen Bonding of Ammonia with (H,OH)-Si(001) Revealed by Experimental and Ab Initio Photoelectron Spectroscopy. <i>Journal of Physical Chemistry A</i> , <b>2020</b> , 124, 5378-5388	2.8	1
11	Theory of Magnetism in Graphitic Materials. Springer Series in Materials Science, <b>2016</b> , 1-24	0.9	1
10	Unidirectional Kondo scattering in layered NbS2. Npj 2D Materials and Applications, 2021, 5,	8.8	1
9	Temperature dependence of quantum oscillations from non-parabolic dispersions. <i>Nature Communications</i> , <b>2021</b> , 12, 6213	17.4	1
8	Modeling Disordered and Nanostructured Graphene <b>2020</b> , 53-72		1
7	Topological Fermi-arc surface resonances in bcc iron. <i>Physical Review B</i> , <b>2020</b> , 102,	3.3	1
6	Structural Phase Transition and Bandgap Control through Mechanical Deformation in Layered Semiconductors 1T日rX2 (X = S, Se) <b>2020</b> , 2, 1115-1120		1
5	Observation of a singular Weyl point surrounded by charged nodal walls in PtGa. <i>Nature Communications</i> , <b>2021</b> , 12, 3994	17.4	1
4	Density Functional Theory Calculations of Topological Insulators <b>2015</b> , 131-160		О
3	Controlling the Quantum Spin Hall Edge States in Two-Dimensional Transition Metal Dichalcogenides. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 6964-6969	6.4	O

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- Magnetization Signature of Topological Surface States in a Non-Symmorphic Superconductor.

  Advanced Materials, **2021**, 33, e2103257

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