Steven G Louie

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7478633/publications.pdf

Version: 2024-02-01

296 papers	60,374 citations	1697 104 h-index	890 242 g-index
304 all docs	304 docs citations	304 times ranked	37495 citing authors

#	Article	IF	Citations
1	Energy Gaps in Graphene Nanoribbons. Physical Review Letters, 2006, 97, 216803.	2.9	4,396
2	Half-metallic graphene nanoribbons. Nature, 2006, 444, 347-349.	13.7	3,878
3	Electron correlation in semiconductors and insulators: Band gaps and quasiparticle energies. Physical Review B, 1986, 34, 5390-5413.	1.1	3,310
4	Discovery of intrinsic ferromagnetism in two-dimensional van der Waals crystals. Nature, 2017, 546, 265-269.	13.7	3,260
5	Relaxation of Crystals with the Quasi-Newton Method. Journal of Computational Physics, 1997, 131, 233-240.	1.9	2,389
6	Recent Advances in Two-Dimensional Materials beyond Graphene. ACS Nano, 2015, 9, 11509-11539.	7.3	2,069
7	Giant bandgap renormalization and excitonic effects in a monolayer transition metal dichalcogenide semiconductor. Nature Materials, 2014, 13, 1091-1095.	13.3	1,470
8	Electron-hole excitations and optical spectra from first principles. Physical Review B, 2000, 62, 4927-4944.	1.1	1,453
9	Optical Spectrum of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>: Many-Body Effects and Diversity of Exciton States. Physical Review Letters, 2013, 111, 216805.	2.9	1,275
10	First-Principles Theory of Quasiparticles: Calculation of Band Gaps in Semiconductors and Insulators. Physical Review Letters, 1985, 55, 1418-1421.	2.9	1,208
11	Crossed Nanotube Junctions. Science, 2000, 288, 494-497.	6.0	1,135
12	Quasiparticle Energies and Band Gaps in Graphene Nanoribbons. Physical Review Letters, 2007, 99, 186801.	2.9	1,092
13	Excitonic Effects and Optical Spectra of Single-Walled Carbon Nanotubes. Physical Review Letters, 2004, 92, 077402.	2.9	875
14	Probing excitonic dark states in single-layer tungsten disulphide. Nature, 2014, 513, 214-218.	13.7	835
15	Renormalization of Molecular Electronic Levels at Metal-Molecule Interfaces. Physical Review Letters, 2006, 97, 216405.	2.9	769
16	Electron-Hole Excitations in Semiconductors and Insulators. Physical Review Letters, 1998, 81, 2312-2315.	2.9	768
17	BerkeleyGW: A massively parallel computer package for the calculation of the quasiparticle and optical properties of materials and nanostructures. Computer Physics Communications, 2012, 183, 1269-1289.	3.0	706
18	Electronic mechanism of hardness enhancement in transition-metal carbonitrides. Nature, 1999, 399, 132-134.	13.7	662

#	Article	IF	Citations
19	Topological defects in graphene: Dislocations and grain boundaries. Physical Review B, 2010, 81, .	1.1	659
20	Spatially resolving edge states of chiral grapheneÂnanoribbons. Nature Physics, 2011, 7, 616-620.	6.5	628
21	Electron-phonon interaction using Wannier functions. Physical Review B, 2007, 76, .	1.1	625
22	Direct observation of the layer-dependent electronic structure in phosphorene. Nature Nanotechnology, 2017, 12, 21-25.	15.6	625
23	Anisotropic behaviours of massless DiracÂfermions in graphene under periodicÂpotentials. Nature Physics, 2008, 4, 213-217.	6.5	609
24	Mechanically controlled binary conductance switching of a single-molecule junction. Nature Nanotechnology, 2009, 4, 230-234.	15.6	609
25	Excitonic Effects on the Optical Response of Graphene and Bilayer Graphene. Physical Review Letters, 2009, 103, 186802.	2.9	604
26	Fully collapsed carbon nanotubes. Nature, 1995, 377, 135-138.	13.7	466
27	First direct observation of Dirac fermions inÂgraphite. Nature Physics, 2006, 2, 595-599.	6.5	466
28	Topological band engineering of graphene nanoribbons. Nature, 2018, 560, 204-208.	13.7	452
29	Amineâ^'Gold Linked Single-Molecule Circuits:â€‰ Experiment and Theory. Nano Letters, 2007, 7, 3477-3482.	4.5	447
30	Spin Polarization and Transport of Surface States in the Topological Insulators<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Bi</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi>Se</mml:mi><mml:mn xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Bi</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi>Te</mml:mi><mml:mn First Principles. Physical Review Letters, 2010, 105, 266806.	2.9	424
31	Molecular bandgap engineering of bottom-up synthesized graphene nanoribbon heterojunctions. Nature Nanotechnology, 2015, 10, 156-160.	15.6	414
32	Disorder, Pseudospins, and Backscattering in Carbon Nanotubes. Physical Review Letters, 1999, 83, 5098-5101.	2.9	408
33	New Generation of Massless Dirac Fermions in Graphene under External Periodic Potentials. Physical Review Letters, 2008, 101, 126804.	2.9	370
34	Tunable Magnetism and Half-Metallicity in Hole-Doped Monolayer GaSe. Physical Review Letters, 2015, 114, 236602.	2.9	350
35	Broken symmetry and pseudogaps in ropes of carbon nanotubes. Nature, 1998, 391, 466-468.	13.7	348
36	Excitonic Effects and the Optical Absorption Spectrum of Hydrogenated Si Clusters. Physical Review Letters, 1998, 80, 3320-3323.	2.9	341

#	Article	IF	Citations
37	Ab initiostatic dielectric matrices from the density-functional approach. I. Formulation and application to semiconductors and insulators. Physical Review B, 1987, 35, 5585-5601.	1.1	338
38	Calcium-Decorated Graphene-Based Nanostructures for Hydrogen Storage. Nano Letters, 2010, 10, 793-798.	4.5	331
39	EPW: A program for calculating the electronâ€“phonon coupling using maximally localized Wannier functions. Computer Physics Communications, 2010, 181, 2140-2148.	3.0	324
40	First-principles calculation of the superconducting transition inMgB2within the anisotropic Eliashberg formalism. Physical Review B, 2002, 66, .	1.1	323
41	Theory and computation of hot carriers generated by surface plasmon polaritons in noble metals. Nature Communications, 2015, 6, 7044.	5.8	317
42	Magnetic brightening and control of dark excitons in monolayer WSe2. Nature Nanotechnology, 2017, 12, 883-888.	15.6	315
43	Theory andAbÂInitioCalculation of Radiative Lifetime of Excitons in Semiconducting Carbon Nanotubes. Physical Review Letters, 2005, 95, 247402.	2.9	295
44	Screening and many-body effects in two-dimensional crystals: Monolayer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> Physical Review B, 2016, 93, .	1.1	290
45	Vacancy Hardening and Softening in Transition Metal Carbides and Nitrides. Physical Review Letters, 2001, 86, 3348-3351.	2.9	284
46	GW100: Benchmarking G₀W₀ for Molecular Systems. Journal of Chemical Theory and Computation, 2015, 11, 5665-5687.	2.3	280
47	Ab initiocalculation of the electronic and optical properties of solid pentacene. Physical Review B, 2003, 67, .	1.1	276
48	Excitonic Effects in the Optical Spectra of Graphene Nanoribbons. Nano Letters, 2007, 7, 3112-3115.	4.5	254
49	Electron Beam Supercollimation in Graphene Superlattices. Nano Letters, 2008, 8, 2920-2924.	4.5	253
50	Electron-Phonon Renormalization of the Direct Band Gap of Diamond. Physical Review Letters, 2010, 105, 265501.	2.9	241
51	Topological Phases in Graphene Nanoribbons: Junction States, Spin Centers, and Quantum Spin Chains. Physical Review Letters, 2017, 119, 076401.	2.9	235
52	Gate-controlled ionization and screening of cobalt adatoms on a graphene surface. Nature Physics, 2011, 7, 43-47.	6.5	233
53	Observing Atomic Collapse Resonances in Artificial Nuclei on Graphene. Science, 2013, 340, 734-737.	6.0	223
54	Site-Specific Substitutional Boron Doping of Semiconducting Armchair Graphene Nanoribbons. Journal of the American Chemical Society, 2015, 137, 8872-8875.	6.6	213

#	Article	IF	Citations
55	Quasiparticle Band Gap of ZnO: High Accuracy from the Conventional<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mml:msup><mml:msup><mml:mi>W</mml:mi><mml:mn> Physical Review Letters, 2010, 105, 146401.	2.9	212
56	AbÂInitioStudy of Hot Carriers in the First Picosecond after Sunlight Absorption in Silicon. Physical Review Letters, 2014, 112, 257402.	2.9	203
57	High thermoelectric power factor in two-dimensional crystals of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Mo</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2017, 95, .	1.1	201
58	Many-body interactions in quasi-freestanding graphene. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 11365-11369.	3.3	200
59	Nonanalyticity, Valley Quantum Phases, and Lightlike Exciton Dispersion in Monolayer Transition Metal Dichalcogenides: Theory and First-Principles Calculations. Physical Review Letters, 2015, 115, 176801.	2.9	196
60	Identifying substitutional oxygen as a prolific point defect in monolayer transition metal dichalcogenides. Nature Communications, 2019, 10, 3382.	5.8	196
61	Ab InitioPhotoabsorption Spectra and Structures of Small Semiconductor and Metal Clusters. Physical Review Letters, 1996, 77, 247-250.	2.9	193
62	Excitons and Optical Spectrum of theSi(111)â"(2Ã—1)Surface. Physical Review Letters, 1999, 83, 856-859.	2.9	191
63	Inversion symmetry and bulk Rashba effect in methylammonium lead iodide perovskite single crystals. Nature Communications, 2018, 9, 1829.	5.8	189
64	Velocity Renormalization and Carrier Lifetime in Graphene from the Electron-Phonon Interaction. Physical Review Letters, 2007, 99, 086804.	2.9	183
65	Diameter and chirality dependence of exciton properties in carbon nanotubes. Physical Review B, 2006, 74, .	1.1	179
66	Photoelectron spin-flipping and texture manipulation in a topological insulator. Nature Physics, 2013, 9, 293-298.	6.5	176
67	High Accuracy Many-Body Calculational Approaches for Excitations in Molecules. Physical Review Letters, 2001, 86, 472-475.	2.9	169
68	Si-O-Si bond-angle distribution in vitreous silica from first-principles29SiNMR analysis. Physical Review B, 2000, 62, R4786-R4789.	1.1	167
69	Atomically precise graphene nanoribbon heterojunctions from a single molecular precursor. Nature Nanotechnology, 2017, 12, 1077-1082.	15.6	162
70	Three-Dimensional Spirals of Atomic Layered MoS₂. Nano Letters, 2014, 14, 6418-6423.	4.5	161
71	Self-consistent pseudopotential method for localized configurations: Molecules. Physical Review B, 1975, 12, 5575-5579.	1.1	160
72	Negative Differential Resistance in Carbon Atomic Wire-Carbon Nanotube Junctions. Nano Letters, 2008, 8, 2900-2905.	4.5	160

#	Article	IF	Citations
73	Structural forms of cubicBC2N. Physical Review B, 2001, 64, .	1.1	159
74	Small phonon contribution to the photoemission kink in the copper oxide superconductors. Nature, 2008, 452, 975-978.	13.7	157
75	Electronâ˜Phonon Interactions in Graphene, Bilayer Graphene, and Graphite. Nano Letters, 2008, 8, 4229-4233.	4.5	156
76	Environmental Screening Effects in 2D Materials: Renormalization of the Bandgap, Electronic Structure, and Optical Spectra of Few-Layer Black Phosphorus. Nano Letters, 2017, 17, 4706-4712.	4.5	155
77	Making Massless Dirac Fermions from a Patterned Two-Dimensional Electron Gas. Nano Letters, 2009, 9, 1793-1797.	4.5	151
78	Coulomb-hole summations and energies for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>calculations with limited number of empty orbitals: A modified static remainder approach. Physical Review B, 2013, 87, .	1.1	149
79	Calcium-decorated carbon nanotubes for high-capacity hydrogen storage: First-principles calculations. Physical Review B, 2009, 80, .	1.1	148
80	Phonon-Assisted Optical Absorption in Silicon from First Principles. Physical Review Letters, 2012, 108, 167402.	2.9	143
81	Landau Levels and Quantum Hall Effect in Graphene Superlattices. Physical Review Letters, 2009, 103, 046808.	2.9	137
82	Excitonic effects in the optical properties of a SiC sheet and nanotubes. Physical Review B, 2011, 84, .	1.1	136
83	Probing the Role of Interlayer Coupling and Coulomb Interactions on Electronic Structure in Few-Layer MoSe₂ Nanostructures. Nano Letters, 2015, 15, 2594-2599.	4.5	136
84	Low Energy Properties of(n,n)Carbon Nanotubes. Physical Review Letters, 1997, 78, 4245-4248.	2.9	129
85	Structural and electronic properties ofn-doped andp-dopedSrTiO3. Physical Review B, 2004, 70, .	1.1	127
86	Inducing metallicity in graphene nanoribbons via zero-mode superlattices. Science, 2020, 369, 1597-1603.	6.0	127
87	Tunable excitons in bilayer graphene. Science, 2017, 358, 907-910.	6.0	126
88	Strong correlations and orbital texture in single-layer 1T-TaSe2. Nature Physics, 2020, 16, 218-224.	6.5	126
89	Mechanical Instability and Ideal Shear Strength of Transition Metal Carbides and Nitrides. Physical Review Letters, 2001, 87, 075503.	2.9	122
90	GW method with the self-consistent Sternheimer equation. Physical Review B, 2010, 81, .	1.1	122

#	Article	IF	Citations
91	Large Spin-Orbit Splitting of Deep In-Gap Defect States of Engineered Sulfur Vacancies in Monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>WS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn><mml:mn> Physical Review Letters, 2019, 123, 076801.	2.9	120
92	Temperature Dependence of the Band Gap of Semiconducting Carbon Nanotubes. Physical Review Letters, 2005, 94, 036801.	2.9	119
93	Bottom-Up Synthesis of N = 13 Sulfur-Doped Graphene Nanoribbons. Journal of Physical Chemistry C, 2016, 120, 2684-2687.	1.5	119
94	Quasiparticle effects in the bulk and surface-state bands of Bi<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Se<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>and Bi<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:	1.1	118
95	Imaging moirÃ© flat bands in three-dimensional reconstructed WSe2/WS2 superlattices. Nature Materials, 2021, 20, 945-950.	13.3	118
96	Self-Consistent Pseudopotential Calculation for a Metal-Semiconductor Interface. Physical Review Letters, 1975, 35, 866-869.	2.9	116
97	Self-Consistent Pseudopotential Calculations on Si(111) Unreconstructed and (2Ã—1) Reconstructed Surfaces. Physical Review Letters, 1975, 34, 1385-1388.	2.9	116
98	Theory of magnetic edge states in chiral graphene nanoribbons. Physical Review B, 2011, 84, .	1.1	113
99	Optimization of metal dispersion in doped graphitic materials for hydrogen storage. Physical Review B, 2008, 78, .	1.1	111
100	Computational design of direct-bandgap semiconductors that lattice-match silicon. Nature, 2001, 409, 69-71.	13.7	110
101	NMR Chemical Shifts of Ice and Liquid Water:Â The Effects of Condensation. Journal of the American Chemical Society, 2000, 122, 123-129.	6.6	109
102	Defect-Induced Modification of Low-Lying Excitons and Valley Selectivity in Monolayer Transition Metal Dichalcogenides. Physical Review Letters, 2018, 121, 167402.	2.9	109
103	Observation of Carrier-Density-Dependent Many-Body Effects in Graphene via Tunneling Spectroscopy. Physical Review Letters, 2010, 104, 036805.	2.9	106
104	Bound Excitons in Metallic Single-Walled Carbon Nanotubes. Nano Letters, 2007, 7, 1626-1630.	4.5	105
105	Ab initio study of hot electrons in GaAs. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 5291-5296.	3.3	104
106	Quasiparticle excitation spectrum for nearly-free-electron metals. Physical Review B, 1989, 39, 8198-8208.	1.1	103
107	Ab initiostudy of silicon in theR8phase. Physical Review B, 1997, 56, 6662-6668.	1.1	103
108	Theory of sodium ordering inNaxCoO2. Physical Review B, 2005, 71, .	1.1	102

#	Article	IF	Citations
109	Angle-Resolved Photoemission Spectra of Graphene from First-Principles Calculations. Nano Letters, 2009, 9, 4234-4239.	4.5	102
110	Physical origin of giant excitonic and magneto-optical responses in two-dimensional ferromagnetic insulators. Nature Communications, 2019, 10, 2371.	5.8	101
111	Quasiparticle band structure of ZnS and ZnSe. Physical Review B, 2002, 66, .	1.1	99
112	Structural Deformation and Intertube Conductance of Crossed Carbon Nanotube Junctions. Physical Review Letters, 2001, 86, 688-691.	2.9	98
113	Graphene Dirac fermions in one-dimensional inhomogeneous field profiles: Transforming magnetic to electric field. Physical Review B, 2010, 81, .	1.1	98
114	Physical Origin of Satellites in Photoemission of Doped Graphene: AnAb InitioGWPlus Cumulant Study. Physical Review Letters, 2013, 110, 146801.	2.9	97
115	A dielectric-defined lateral heterojunction in a monolayer semiconductor. Nature Electronics, 2019, 2, 60-65.	13.1	95
116	Klein tunneling and supercollimation of pseudospin-1 electromagnetic waves. Physical Review B, 2016, 93, .	1.1	93
117	Direct measurement of quantum phases in graphene via photoemission spectroscopy. Physical Review B, 2011, 84, .	1.1	91
118	Spin splitting of dopant edge state in magnetic zigzag graphene nanoribbons. Nature, 2021, 600, 647-652.	13.7	91
119	Spin Polarization of Photoelectrons from Topological Insulators. Physical Review Letters, 2012, 109, 097601.	2.9	89
120	Excitons and Optical Properties ofÎ±-Quartz. Physical Review Letters, 2000, 85, 2613-2616.	2.9	88
121	Hydrostatic pressure effects on the structural and electronic properties of carbon nanotubes. Physica Status Solidi (B): Basic Research, 2004, 241, 3352-3359.	0.7	88
122	Tuning charge and correlation effects for a single molecule on a graphene device. Nature Communications, 2016, 7, 13553.	5.8	82
123	Tunable Excitons in Biased Bilayer Graphene. Nano Letters, 2010, 10, 426-431.	4.5	81
124	First-principles<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>DFT</mml:mi><mml:mo>+</mml:mo><mml:mi>G</mml:mi><mml:r of oxygen vacancies in rutile<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>TiO</mml:mtext><mml:mn>2</mml:mn></mml:msub> Physical Review B, 2014, 89, .	1.1	80
125	Nonuniform sampling schemes of the Brillouin zone for many-electron perturbation-theory calculations in reduced dimensionality. Physical Review B, 2017, 95, .	1.1	78
126	Doping effects on the electronic and structural properties ofCoO2: AnLSDA+Ustudy. Physical Review B, 2004, 70, .	1.1	77

#	Article	IF	Citations
127	Structural and electronic properties of carbon in hybrid diamond-graphite structures. Physical Review B, 2005, 72, .	1.1	77
128	Bottom-up Assembly of Nanoporous Graphene with Emergent Electronic States. Journal of the American Chemical Society, 2020, 142, 13507-13514.	6.6	77
129	Hierarchical On-Surface Synthesis of Graphene Nanoribbon Heterojunctions. ACS Nano, 2018, 12, 2193-2200.	7.3	75
130	Ultrasensitive tunability of the direct bandgap of 2D InSe flakes via strain engineering. 2D Materials, 2018, 5, 021002.	2.0	75
131	Theory of semiconductor surface states and metalâ€“semiconductor interfaces. Journal of Vacuum Science and Technology, 1976, 13, 790-797.	1.9	74
132	Tuning Many-Body Interactions in Graphene: The Effects of Doping on Excitons and Carrier Lifetimes. Physical Review Letters, 2014, 112, .	2.9	74
133	Evidence for quantum spin liquid behaviour in single-layer 1T-TaSe2 from scanning tunnelling microscopy. Nature Physics, 2021, 17, 1154-1161.	6.5	74
134	Large electronâ€“phonon interactions from FeSe phonons in a monolayer. New Journal of Physics, 2015, 17, 073027.	1.2	73
135	Direct observation of Klein tunneling in phononic crystals. Science, 2020, 370, 1447-1450.	6.0	73
136	First-Principles Study of Electron Linewidths in Graphene. Physical Review Letters, 2009, 102, 076803.	2.9	72
137	Gate Switchable Transport and Optical Anisotropy in 90Â° Twisted Bilayer Black Phosphorus. Nano Letters, 2016, 16, 5542-5546.	4.5	71
138	Spectral functions of the uniform electron gas via coupled-cluster theory and comparison to the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m related approximations. Physical Review B, 2016, 93, .	1.1	70
139	Method: Correlation-Enhanced Interactions and Superconductivity in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>	2.9	70
140	Evaluation of quasiparticle energies for semiconductors without inversion symmetry. Physical Review B, 1989, 40, 3162-3168.	1.1	69
141	Systematic determination of absolute absorption cross-section of individual carbon nanotubes. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 7564-7569.	3.3	69
142	Exchange-driven intravalley mixing of excitons in monolayer transition metal dichalcogenides. Nature Physics, 2019, 15, 228-232.	6.5	68
143	Phonon Softening and Superconductivity in Tellurium under Pressure. Physical Review Letters, 1996, 77, 1151-1154.	2.9	67
144	Hypothetical hard structures of carbon with cubic symmetry. Physical Review B, 2006, 74, .	1.1	66

#	Article	IF	Citations
145	Ab initioNMR Chemical Shift of Diamond, Chemical-Vapor-Deposited Diamond, and Amorphous Carbon. Physical Review Letters, 1997, 79, 2340-2343.	2.9	65
146	NMR Chemical Shifts in Hard Carbon Nitride Compounds. Physical Review Letters, 1998, 80, 3388-3391.	2.9	65
147	Quasiparticle energy of semicoredelectrons inZnS: CombinedLDA+UandGWapproach. Physical Review B, 2006, 74, .	1.1	65
148	Enhanced electron-hole interaction and optical absorption in a silicon nanowire. Physical Review B, 2007, 75, .	1.1	65
149	Predominance of non-adiabatic effects in zero-point renormalization of the electronic band gap. Npj Computational Materials, 2020, 6, .	3.5	65
150	Electronâ^'Hole Interaction in Carbon Nanotubes: Novel Screening and Exciton Excitation Spectra. Nano Letters, 2009, 9, 1330-1334.	4.5	64
151	Orbitally Matched Edge-Doping in Graphene Nanoribbons. Journal of the American Chemical Society, 2018, 140, 807-813.	6.6	64
152	Anomalous Quasiparticle Lifetime in Graphite: Band Structure Effects. Physical Review Letters, 2001, 87, 246405.	2.9	62
153	Comparing time-dependent density functional theory with many-body perturbation theory for semiconductors: Screened range-separated hybrids and the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m plus Bethe-Salpeter approach. Physical Review Materials, 2019, 3, .	2.9	61
154	Discovering and understanding materials through computation. Nature Materials, 2021, 20, 728-735.	13.3	60
155	Coexistence of sharp quasiparticle dispersions and disorder features in graphite. Physical Review B, 2005, 71, .	1.1	59
156	Quasiparticle electronic structure of bismuth telluride in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:math>approximation. Physical Review B, 2010, 82, .	1.1	59
157	Coupling of Nonlocal Potentials to Electromagnetic Fields. Physical Review Letters, 2001, 87, 087402.	2.9	56
158	Ab initioelectronic relaxation times and transport in noble metals. Physical Review B, 2016, 94, .	1.1	56
159	Origins of Singlet Fission in Solid Pentacene from an abÂinitio Greenâ€™s Function Approach. Physical Review Letters, 2017, 119, 267401.	2.9	55
160	Topological Phases in Cove-Edged and Chevron Graphene Nanoribbons: Geometric Structures, Z₂ Invariants, and Junction States. Nano Letters, 2018, 18, 7247-7253.	4.5	55
161	Negative Differential Resistance in Transport through Organic Molecules on Silicon. Physical Review Letters, 2007, 98, 066807.	2.9	54
162	Quasiparticle Excitations and Charge Transition Levels of Oxygen Vacancies in Hafnia. Physical Review Letters, 2011, 107, 216803.	2.9	54

#	Article	IF	Citations
163	First-principles scattering-state approach for nonlinear electrical transport in nanostructures. Physical Review B, 2007, 76, .	1.1	53
164	Mechanism for optical initialization of spin in NV<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mrow /><mml:mo>â^’</mml:mo></mml:msup></mml:math>center in diamond. Physical Review B, 2012, 86, .	1.1	53
165	Excitation spectra of aromatic molecules within a real-space<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math> formalism: Role of self-consistency and vertex corrections. Physical Review B, 2016, 94, .	1.1	53
166	Universal slow plasmons and giant field enhancement in atomically thin quasi-two-dimensional metals. Nature Communications, 2020, 11, 1013.	5.8	53
167	Generation of Anisotropic Massless Dirac Fermions and Asymmetric Klein Tunneling in Few-Layer Black Phosphorus Superlattices. Nano Letters, 2017, 17, 2280-2286.	4.5	52
168	Unifying Optical Selection Rules for Excitons in Two Dimensions: Band Topology and Winding Numbers. Physical Review Letters, 2018, 120, 087402.	2.9	52
169	Rational Passivation of Sulfur Vacancy Defects in Two-Dimensional Transition Metal Dichalcogenides. ACS Nano, 2021, 15, 8780-8789.	7.3	52
170	GW approach to Anderson model out of equilibrium: Coulomb blockade and false hysteresis in theIâ^’Vcharacteristics. Physical Review B, 2009, 79, .	1.1	51
171	Van Hove singularity and apparent anisotropy in the electron-phonon interaction in graphene. Physical Review B, 2008, 77, .	1.1	50
172	Formation and Dynamics of Electron-Irradiation-Induced Defects in Hexagonal Boron Nitride at Elevated Temperatures. Nano Letters, 2016, 16, 7142-7147.	4.5	49
173	Selection rules for one- and two-photon absorption by excitons in carbon nanotubes. Physical Review B, 2006, 73, .	1.1	48
174	Ab initioGWquasiparticle energies of small sodium clusters by an all-electron mixed-basis approach. Physical Review B, 2001, 63, .	1.1	46
175	Ab initio GWquasiparticle calculation of small alkali-metal clusters. Physical Review B, 2002, 65, .	1.1	46
176	Electromagnetic screening by metals. American Journal of Physics, 1988, 56, 989-992.	0.3	45
177	Ab initiocalculation of band-gap renormalization in highly excited GaAs. Physical Review B, 2004, 69, .	1.1	45
178	Molecular Self-Assembly in a Poorly Screened Environment: F₄TCNQ on Graphene/BN. ACS Nano, 2015, 9, 12168-12173.	7.3	45
179	Electron-phonon coupling in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>C</mml:mtext><mml:mrow><mml:mn>60</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> hybrid functionals. Physical Review B, 2010, 81, .	1.1	43
180	Satellite band structure in silicon caused by electron-plasmon coupling. Physical Review B, 2015, 91, .	1.1	43

#	Article	IF	Citations
181	Anomalous insulator-metal transition in boron nitride-graphene hybrid atomic layers. Physical Review B, 2012, 86, .	1.1	42
182	Tuning two-dimensional band structure of Cu(111) surface-state electrons that interplay with artificial supramolecular architectures. Physical Review B, 2013, 88, .	1.1	42
183	Large enhancement of boron solubility in silicon due to biaxial stress. Applied Physics Letters, 2002, 80, 4738-4740.	1.5	41
184	Orbital Symmetry and the Optical Response of Single-Layer MX Monochalcogenides. Nano Letters, 2018, 18, 1925-1929.	4.5	41
185	Length-Dependent Evolution of Type II Heterojunctions in Bottom-Up-Synthesized Graphene Nanoribbons. Nano Letters, 2019, 19, 3221-3228.	4.5	41
186	Theory of exciton-phonon coupling. Physical Review B, 2022, 105, .	1.1	40
187	Imaging and Tuning Molecular Levels at the Surface of a Gated Graphene Device. ACS Nano, 2014, 8, 5395-5401.	7.3	39
188	Temperature-Induced Topological Phase Transitions: Promoted versus Suppressed Nontrivial Topology. Physical Review Letters, 2016, 117, 246401.	2.9	39
189	Manipulation and Characterization of Aperiodical Graphene Structures Created in a Two-Dimensional Electron Gas. Physical Review Letters, 2014, 113, 196803.	2.9	36
190	Reproducibility in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e1825" altimg="si271.svg"><mml:mrow><mml:msub><mml:mrow><mml:mi>G</mml:mi></mml:mrow><mml:mrow><mml:mn>0</mml:mn></ calculations for solids. Computer Physics Communications, 2020, 255, 107242.	3.0	36
191	Giant exciton-enhanced shift currents and direct current conduction with subbandgap photo excitations produced by many-electron interactions. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	36
192	Imaging local discharge cascades for correlated electrons in WS2/WSe2 moirÃ© superlattices. Nature Physics, 2021, 17, 1114-1119.	6.5	36
193	Excitons in carbon nanotubes: Diameter and chirality trends. Physica Status Solidi (B): Basic Research, 2007, 244, 4016-4020.	0.7	35
194	Prediction of superconducting properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CaB</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms anisotropic Eliashberg theory. Physical Review B, 2009, 80, .	1.1	35
195	Low-lying excited states in crystalline perylene. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 284-289.	3.3	35
196	Large-scale GW calculations on pre-exascale HPC systems. Computer Physics Communications, 2019, 235, 187-195.	3.0	35
197	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>quasiparticle corrections to the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>LDA</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi><mml:mo>âˆ•</mml:mo><mml:m structure of bcc hydrogen. Physical Review B, 2008, 77, .	1.1	34
198	Valley-dependent exciton fine structure and Autlerâ€“Townes doublets from Berry phases in monolayer MoSe2. Nature Materials, 2019, 18, 1065-1070.	13.3	34

#	Article	IF	Citations
199	Accelerating GW-Based Energy Level Alignment Calculations for Moleculeâ€“Metal Interfaces Using a Substrate Screening Approach. Journal of Chemical Theory and Computation, 2019, 15, 4218-4227.	2.3	34
200	Automated construction of maximally localized Wannier functions: Optimized projection functions method. Physical Review B, 2015, 92, .	1.1	33
201	Concentration Dependence of Dopant Electronic Structure in Bottom-up Graphene Nanoribbons. Nano Letters, 2018, 18, 3550-3556.	4.5	31
202	Tuning colour centres at a twisted hexagonal boron nitride interface. Nature Materials, 2022, 21, 896-902.	13.3	31
203	Spectroscopy of zigzag single-walled carbon nanotubes: Comparing femtosecond transient absorption spectra withab initiocalculations. Physical Review B, 2006, 74, .	1.1	29
204	Electronic and optical properties of body-centered-tetragonal Si and Ge. Physical Review B, 2010, 81, .	1.1	29
205	First-Principles Calculations of Quasiparticle Excitations of Open-Shell Condensed Matter Systems. Physical Review Letters, 2012, 109, 036406.	2.9	29
206	Narrow-band high-lying excitonsÂwith negative-mass electrons in monolayer WSe2. Nature Communications, 2021, 12, 5500.	5.8	29
207	Anisotropic Eliashberg theory and the two-band model for the superconducting properties ofMgB2. Physical Review B, 2006, 73, .	1.1	27
208	Ab initiocalculations of pressure-induced structural phase transitions of GeTe. Physical Review B, 2010, 82, .	1.1	27
209	Anomalous Anderson localization behaviors in disordered pseudospin systems. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 4087-4092.	3.3	27
210	Momentum-Resolved Dielectric Response of Free-Standing Mono-, Bi-, and Trilayer Black Phosphorus. Nano Letters, 2019, 19, 8303-8310.	4.5	27
211	Covalent Câ€“N Bond Formation through a Surface Catalyzed Thermal Cyclodehydrogenation. Journal of the American Chemical Society, 2020, 142, 3696-3700.	6.6	27
212	Topology Classification using Chiral Symmetry and Spin Correlations in Graphene Nanoribbons. Nano Letters, 2021, 21, 197-202.	4.5	27
213	Ab initioquasiparticle band structure of ABA and ABC-stacked graphene trilayers. Physical Review B, 2014, 89, .	1.1	26
214	Band gap renormalization, carrier mobilities, and the electron-phonon self-energy in crystalline naphthalene. Physical Review B, 2020, 101, .	1.1	26
215	Theoretical Models for the Optical Properties of Clusters and Nanostructures. International Journal of Modern Physics B, 1997, 11, 2727-2776.	1.0	25
216	Quasiparticle properties of a simple metal at high electron temperatures. Physical Review B, 2002, 66, .	1.1	24

#	Article	IF	Citations
217	Effects of self-consistency and plasmon-pole models on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math> for closed-shell molecules. Physical Review B, 2014, 90, .	3.7	24
218	Electron Supercollimation in Graphene and Dirac Fermion Materials Using One-Dimensional Disorder Potentials. Physical Review Letters, 2014, 113, 026802.	2.9	24
219	Total energy method for solids and solid surfaces. International Journal of Quantum Chemistry, 1984, 26, 105-120.	1.0	23
220	Selective functionalization of halogens on zigzag graphene nanoribbons: A route to the separation of zigzag graphene nanoribbons. Applied Physics Letters, 2010, 97, 233101.	1.5	23
221	Enhanced electron-phonon coupling near the lattice instability of superconducting NbC<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>N<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math> from density-functional calculations. Physical Review B, 2011, 84, .	1.1	23
222	Mechanism for bias-assisted indium mass transport on carbon nanotube surfaces. Physical Review B, 2005, 72, .	1.1	22
223	New Dirac Fermions in Periodically Modulated Bilayer Graphene. Nano Letters, 2011, 11, 2596-2600.	4.5	22
224	Dynamics of Symmetry-Breaking Stacking Boundaries in Bilayer MoS₂. Journal of Physical Chemistry C, 2017, 121, 22559-22566.	1.5	22
225	Rationally Designed Topological Quantum Dots in Bottom-Up Graphene Nanoribbons. ACS Nano, 2021, 15, 20633-20642.	7.3	22
226	Bound excitons and optical properties of bulktrans-polyacetylene. Physical Review B, 2004, 70, .	1.1	21
227	Optical Imaging and Spectroscopy of Atomically Precise Armchair Graphene Nanoribbons. Nano Letters, 2020, 20, 1124-1130.	4.5	21
228	Topological Phases in Graphene Nanoribbons Tuned by Electric Fields. Physical Review Letters, 2021, 127, 166401.	2.9	20
229	Unconventional excitonic states with phonon sidebands in layered silicon diphosphide. Nature Materials, 2022, 21, 773-778.	13.3	20
230	Reply to â€œComment on â€˜First-principles calculation of the superconducting transition inMgB2within the anisotropic Eliashberg formalismâ€™ â€• Physical Review B, 2004, 69, .	1.1	19
231	Nanoparticles behaving oddly. Nature, 1996, 384, 612-613.	13.7	17
232	Anisotropic Eliashberg theory for superconductivity in compressed and doped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>MgB</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2009, 79, .	1.1	17
233	Theory of the electronic and transport properties of graphene under a periodic electric or magnetic field. Physica E: Low-Dimensional Systems and Nanostructures, 2011, 43, 651-656.	1.3	17
234	Electron transport and optical properties of carbon nanostructures from first principles. Computer Physics Communications, 2005, 169, 1-8.	3.0	16

#	Article	IF	Citations
235	Electrostatically Driven Nanoballoon Actuator. Nano Letters, 2016, 16, 6787-6791.	4.5	16
236	Proposal for a bulk material based on a monolayer FeSe on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></m superconductor. Physical Review B, 2016, 93, .	1.1	16
237	Effective mass in bilayer graphene at low carrier densities: The role of potential disorder and electron-electron interaction. Physical Review B, 2016, 94, .	1.1	16
238	Unmasking the Origin of Kinks in the Photoemission Spectra of Cuprate Superconductors. Physical Review Letters, 2021, 126, 146401.	2.9	16
239	Numerical integration for ab initio many-electron self energy calculations within the GW approximation. Journal of Computational Physics, 2015, 286, 1-13.	1.9	15
240	Dispersion and line shape of plasmon satellites in one, two, and three dimensions. Physical Review B, 2016, 93, .	1.1	15
241	Quasiparticle band structure of lanthanum hydride. Physical Review B, 2001, 64, .	1.1	14
242	Improved quasiparticle wave functions and mean field for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mml:msub><mml:m Initialization with the COHSEX operator. Physical Review B, 2014, 90, .	1.1	14
243	Low rank approximation in G 0 W 0 calculations. Science China Mathematics, 2016, 59, 1593-1612.	0.8	14
244	Geometry and electronic structure of iridium adsorbed on graphene. Physical Review B, 2019, 99, .	1.1	14
245	First-principles theory of electron-spin fluctuation coupling and superconducting instabilities in iron selenide. Physical Review B, 2015, 91, .	1.1	13
246	Static subspace approximation for the evaluation of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mml:msub><mml:m quasiparticle energies within a sum-over-bands approach. Physical Review B, 2019, 99, .	1.1	13
247	Pseudospin-1 Physics of Photonic Crystals. Research, 2019, 2019, 3054062.	2.8	13
248	Theory of metastable group-IV alloys formed from CVD precursors. Physical Review B, 2001, 64, .	1.1	12
249	First-principles studies of the electronic structure of cyclopentene on Si(001): density functional theory and GW calculations. Physica Status Solidi (B): Basic Research, 2006, 243, 2048-2053.	0.7	12
250	Contact dependence of the conductance of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>molecular junctions from first principles. Physical Review B, 2008, 77, .	1.1	12
251	Spontaneous twisting of a collapsed carbon nanotube. Nano Research, 2017, 10, 1942-1949.	5.8	12
252	A Structure Preserving Lanczos Algorithm for Computing the Optical Absorption Spectrum. SIAM Journal on Matrix Analysis and Applications, 2018, 39, 683-711.	0.7	12

#	Article	IF	Citations
253	Insulating titanium oxynitride for visible light photocatalysis. Physical Review B, 2019, 99, .	1.1	12
254	Layer-Dependent Electronic Structure of Atomically Resolved Two-Dimensional Gallium Selenide Telluride. Nano Letters, 2019, 19, 1782-1787.	4.5	12
255	A molecular shift register made using tunable charge patterns in one-dimensional molecular arrays on graphene. Nature Electronics, 2020, 3, 598-603.	13.1	12
256	Optical and magneto-optical properties of ferromagnetic monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CrBr</mml:mi><mml:mn>3</mml:mn></mml:msub></mm : A first-principles <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m	0.9	12
257	Vibrational properties of single walled carbon nanotubes under pressure from Raman scattering experiments and molecular dynamics simulations. Physica Status Solidi (B): Basic Research, 2007, 244, 121-126.	0.7	11
258	Resonant Excitation of GrapheneK-Phonon and Intra-Landau-Level Excitons in Magneto-Optical Spectroscopy. Physical Review Letters, 2012, 108, 247401.	2.9	11
259	Effect of spin fluctuations on quasiparticle excitations: First-principles theory and application to sodium and lithium. Physical Review B, 2014, 89, .	1.1	11
260	Intervalley Excitonic Hybridization, Optical Selection Rules, and Imperfect Circular Dichroism in Monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>h</mml:mi><mml:mtext>â^'</mml:mtext><mml:mi>BN</mml:mi></mml:mrow></mml:math>. Physical Review Letters, 2022, 128, 047402.	2.9	11
261	Pseudo-atomic orbital behavior in graphene nanoribbons with four-membered rings. Science Advances, 2021, 7, eabl5892.	4.7	11
262	Many-body effects in the X-ray absorption spectra of liquid water. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2201258119.	3.3	11
263	Theory of quasiparticle energies: Band gaps and excitation spectra in solids. International Journal of Quantum Chemistry, 1987, 32, 31-44.	1.0	10
264	Alternative structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml with higher energy valence band edge. Physical Review B, 2017, 95, .	1.1	9
265	Symmetry rules shaping spin-orbital textures in surface states. Physical Review B, 2017, 95, .	1.1	9
266	Solving the Bethe-Salpeter equation on a subspace: Approximations and consequences for low-dimensional materials. Physical Review B, 2021, 103, .	1.1	9
267	Nonuniversal critical behavior in disordered pseudospin-1 systems. Physical Review B, 2019, 99, .	1.1	8
268	Electronic Structure and Energetics of MgB2 Nanotube. Journal of the Physical Society of Japan, 2007, 76, 043707.	0.7	7
269	Fermi surfaces and quantum oscillations in the underdoped high-Tcsuperconductors YBa2Cu3O6.5and YBa2Cu4O8. Physical Review B, 2011, 84, .	1.1	7
270	Inelastic carrier lifetime in bilayer graphene. Applied Physics Letters, 2012, 100, .	1.5	7

#	Article	IF	Citations
271	Tunnel-FET Switching Is Governed by Non-Lorentzian Spectral Line Shape. Proceedings of the IEEE, 2020, 108, 1235-1244.	16.4	7
272	Cyclopentadiene stability: Quantum Monte Carlo, coupled cluster, and density functional theory determinations. Molecular Physics, 1999, 96, 629-632.	0.8	6
273	Excitonic Effects and Optical Spectra of Single-Walled Carbon Nanotubes. AIP Conference Proceedings, 2005, , .	0.3	6
274	Intermolecular interactions and substrate effects for an adamantane monolayer on a Au(111) surface. Physical Review B, 2013, 88, .	1.1	6
275	Comparison of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m band structure to semiempirical approach for an FeSe monolayer. Physical Review B, 2020, 101, .	1.1	6
276	Polaron spectral properties in doped ZnO and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></m from first principles. Physical Review Research, 2020, 2, .	1.3	6
277	Quasiparticle energies and optical excitations of 3C-SiC divacancy from <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m plus Bethe-Salpeter equationÂcalculations. Physical Review Materials, 2022, 6, .	0.9	6
278	Quasiparticle energies and dielectric functions of diamond polytypes. Physical Review Materials, 2017, 1, .	0.9	5
279	Automated construction of maximally localized Wannier functions for bands with nontrivial topology. Physical Review B, 2016, 94, .	1.1	4
280	Ab initio Modelling of Plasmons in Metalâ€semiconductor Bilayer Transitionâ€metal Dichalcogenide Heterostructures. Israel Journal of Chemistry, 2017, 57, 540-546.	1.0	4
281	Multiple strong topological gaps and hexagonal warping in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Bi</mml:mi><mml:mn>1</mml:mn></mml:m Physical Review B, 2022, 105, .	1.1	4
282	Theory of the Quasiparticle Effective Masses in Semiconductors based on an Electron Self Energy Approach. Materials Research Society Symposia Proceedings, 1990, 193, 113.	0.1	3
283	FIRST-PRINCIPLES THEORY OF ELECTRON EXCITATION ENERGIES IN SOLIDS, SURFACES, AND DEFECTS. , 1998, , 96-142.		3
284	Low-energy structures of K atoms in expandedK3C60monolayers:Ab initiopseudopotential density-functional calculations. Physical Review B, 2008, 77, .	1.1	3
285	SU(4) symmetry breaking revealed by magneto-optical spectroscopy in epitaxial graphene. Physical Review B, 2015, 91, .	1.1	2
286	Real-space study of the optical absorption in alternative phases of silicon. Physical Review Materials, 2017, 1, .	0.9	2
287	Electronic structure and quantum conductance of nanotube structures: Defects, crossed-tube junctions, and nanopeapods. AIP Conference Proceedings, 2001, , .	0.3	1
288	Excitonic Dark States in Single Atomic Layer of Transition Metal Dichalcogenide. , 2014, , .		1

#	Article	IF	Citations
289	Electronic Structure of Graphite Intercalation Compounds. Materials Research Society Symposia Proceedings, 1982, 20, 107.	0.1	0
290	Variational Quantum Monte Carlo Calculation of Materials Properties. Materials Research Society Symposia Proceedings, 1988, 141, 3.	0.1	0
291	Tight-Binding Formalism for Ionic Fullerides and its Application to Alkali-C60 Polymers. Materials Research Society Symposia Proceedings, 1997, 491, 395.	0.1	0
292	First-Principles Study of Optical Excitations in Alpha Quartz. Materials Research Society Symposia Proceedings, 1999, 579, 3.	0.1	0
293	Temperature and Hydrostatic Pressure Effects on the Band Gap of Semiconducting Carbon Nanotubes. AIP Conference Proceedings, 2005, , .	0.3	0
294	Family Behavior of the Pressure and Temperature Dependences of the Band Gap of Semiconducting Carbon Nanotubes. AIP Conference Proceedings, 2005, , .	0.3	0
295	Spatially Dependent Inelastic Tunneling in Gd@C82. AIP Conference Proceedings, 2005, , .	0.3	0
296	Band offsets in c-Si/Si-XII heterojunctions. Solid State Communications, 2014, 191, 6-9.	0.9	0