

# Steven G Louie

## List of Publications by Year in descending order

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296  
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citing authors

#	ARTICLE	IF	CITATIONS
1	Intervalley Excitonic Hybridization, Optical Selection Rules, and Imperfect Circular Dichroism in Monolayer $\text{BN}$ . <i>Physical Review Letters</i> , 2021, 126, 146401.	7.8	11
2	Optical and magneto-optical properties of ferromagnetic monolayer $\text{CrBr}_3$ : A first-principles calculation. <i>Physical Review Materials</i> , 2022, 6, .	2.4	12
3	Theory of exciton-phonon coupling. <i>Physical Review B</i> , 2022, 105, .	3.2	40
4	Multiple strong topological gaps and hexagonal warping in $\text{Bi}_2\text{Te}_3$ . <i>Physical Review B</i> , 2022, 105, .	4.2	41
5	Quasiparticle energies and optical excitations of 3C-SiC divacancy from $\text{GW}$ plus Bethe-Salpeter equation calculations. <i>Physical Review Materials</i> , 2022, 6, .	2.4	6
6	Many-body effects in the X-ray absorption spectra of liquid water. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, e2201258119.	7.1	11
7	Unconventional excitonic states with phonon sidebands in layered silicon diphosphide. <i>Nature Materials</i> , 2022, 21, 773-778.	27.5	20
8	Tuning colour centres at a twisted hexagonal boron nitride interface. <i>Nature Materials</i> , 2022, 21, 896-902.	27.5	31
9	Topology Classification using Chiral Symmetry and Spin Correlations in Graphene Nanoribbons. <i>Nano Letters</i> , 2021, 21, 197-202.	9.1	27
10	Solving the Bethe-Salpeter equation on a subspace: Approximations and consequences for low-dimensional materials. <i>Physical Review B</i> , 2021, 103, .	3.2	9
11	Imaging moiré flat bands in three-dimensional reconstructed $\text{WSe}_2/\text{WS}_2$ superlattices. <i>Nature Materials</i> , 2021, 20, 945-950.	27.5	118
12	Unmasking the Origin of Kinks in the Photoemission Spectra of Cuprate Superconductors. <i>Physical Review Letters</i> , 2021, 126, 146401.	7.8	16
13	Discovering and understanding materials through computation. <i>Nature Materials</i> , 2021, 20, 728-735.	27.5	60
14	Rational Passivation of Sulfur Vacancy Defects in Two-Dimensional Transition Metal Dichalcogenides. <i>ACS Nano</i> , 2021, 15, 8780-8789.	14.6	52
15	Giant exciton-enhanced shift currents and direct current conduction with subbandgap photo excitations produced by many-electron interactions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	7.1	36
16	Evidence for quantum spin liquid behaviour in single-layer 1T-TaSe <sub>2</sub> from scanning tunnelling microscopy. <i>Nature Physics</i> , 2021, 17, 1154-1161.	16.7	74
17	Imaging local discharge cascades for correlated electrons in $\text{WS}_2/\text{WSe}_2$ moiré superlattices. <i>Nature Physics</i> , 2021, 17, 1114-1119.	16.7	36
18	Narrow-band high-lying excitons with negative-mass electrons in monolayer $\text{WSe}_2$ . <i>Nature Communications</i> , 2021, 12, 5500.	12.8	29

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19	Topological Phases in Graphene Nanoribbons Tuned by Electric Fields. <i>Physical Review Letters</i> , 2021, 127, 166401.	7.8	20
20	Rationally Designed Topological Quantum Dots in Bottom-Up Graphene Nanoribbons. <i>ACS Nano</i> , 2021, 15, 20633-20642.	14.6	22
21	Spin splitting of dopant edge state in magnetic zigzag graphene nanoribbons. <i>Nature</i> , 2021, 600, 647-652.	27.8	91
22	Pseudo-atomic orbital behavior in graphene nanoribbons with four-membered rings. <i>Science Advances</i> , 2021, 7, eabl5892.	10.3	11
23	Tunnel-FET Switching Is Governed by Non-Lorentzian Spectral Line Shape. <i>Proceedings of the IEEE</i> , 2020, 108, 1235-1244.	21.3	7
24	Optical Imaging and Spectroscopy of Atomically Precise Armchair Graphene Nanoribbons. <i>Nano Letters</i> , 2020, 20, 1124-1130.	9.1	21
25	Strong correlations and orbital texture in single-layer 1T-TaSe <sub>2</sub> . <i>Nature Physics</i> , 2020, 16, 218-224.	16.7	126
26	Inducing metallicity in graphene nanoribbons via zero-mode superlattices. <i>Science</i> , 2020, 369, 1597-1603.	12.6	127
27	Predominance of non-adiabatic effects in zero-point renormalization of the electronic band gap. <i>Npj Computational Materials</i> , 2020, 6, .	8.7	65
28	Comparison of $G$ band structure to semiempirical approach for an FeSe monolayer. <i>Physical Review B</i> , 2020, 101, .	7.5	36
29	Reproducibility in $G$ band calculations for solids. <i>Computer Physics Communications</i> , 2020, 255, 107242.	7.5	36
30	Band gap renormalization, carrier mobilities, and the electron-phonon self-energy in crystalline naphthalene. <i>Physical Review B</i> , 2020, 101, .	3.2	26
31	Bottom-up Assembly of Nanoporous Graphene with Emergent Electronic States. <i>Journal of the American Chemical Society</i> , 2020, 142, 13507-13514.	13.7	77
32	Universal slow plasmons and giant field enhancement in atomically thin quasi-two-dimensional metals. <i>Nature Communications</i> , 2020, 11, 1013.	12.8	53
33	Covalent C-N Bond Formation through a Surface Catalyzed Thermal Cyclodehydrogenation. <i>Journal of the American Chemical Society</i> , 2020, 142, 3696-3700.	13.7	27
34	A molecular shift register made using tunable charge patterns in one-dimensional molecular arrays on graphene. <i>Nature Electronics</i> , 2020, 3, 598-603.	26.0	12
35	Polaron spectral properties in doped ZnO and $SrTiO_3$ from first principles. <i>Physical Review Research</i> , 2020, 2, .	12.6	73
36	Direct observation of Klein tunneling in phononic crystals. <i>Science</i> , 2020, 370, 1447-1450.	12.6	73



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55	Orbital Symmetry and the Optical Response of Single-Layer MX Monochalcogenides. Nano Letters, 2018, 18, 1925-1929.	9.1	41
56	Unifying Optical Selection Rules for Excitons in Two Dimensions: Band Topology and Winding Numbers. Physical Review Letters, 2018, 120, 087402.	7.8	52
57	Hierarchical On-Surface Synthesis of Graphene Nanoribbon Heterojunctions. ACS Nano, 2018, 12, 2193-2200.	14.6	75
58	Low-lying excited states in crystalline perylene. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 284-289.	7.1	35
59	Ultrasensitive tunability of the direct bandgap of 2D InSe flakes via strain engineering. 2D Materials, 2018, 5, 021002.	4.4	75
60	Orbitally Matched Edge-Doping in Graphene Nanoribbons. Journal of the American Chemical Society, 2018, 140, 807-813.	13.7	64
61	Topological Phases in Cove-Edged and Chevron Graphene Nanoribbons: Geometric Structures, $Z_2$ Invariants, and Junction States. Nano Letters, 2018, 18, 7247-7253.	9.1	55
62	Defect-Induced Modification of Low-Lying Excitons and Valley Selectivity in Monolayer Transition Metal Dichalcogenides. Physical Review Letters, 2018, 121, 167402.	7.8	109
63	A Structure Preserving Lanczos Algorithm for Computing the Optical Absorption Spectrum. SIAM Journal on Matrix Analysis and Applications, 2018, 39, 683-711.	1.4	12
64	Concentration Dependence of Dopant Electronic Structure in Bottom-up Graphene Nanoribbons. Nano Letters, 2018, 18, 3550-3556.	9.1	31
65	Inversion symmetry and bulk Rashba effect in methylammonium lead iodide perovskite single crystals. Nature Communications, 2018, 9, 1829.	12.8	189
66	Topological band engineering of graphene nanoribbons. Nature, 2018, 560, 204-208.	27.8	452
67	Nonuniform sampling schemes of the Brillouin zone for many-electron perturbation-theory calculations in reduced dimensionality. Physical Review B, 2017, 95, .	3.2	78
68	Spontaneous twisting of a collapsed carbon nanotube. Nano Research, 2017, 10, 1942-1949.	10.4	12
69	<i>Ab initio</i> Modelling of Plasmons in Metal-semiconductor Bilayer Transition-metal Dichalcogenide Heterostructures. Israel Journal of Chemistry, 2017, 57, 540-546.	2.3	4
70	Alternative structure of $\text{TiO}_2$ with higher energy valence band edge. Physical Review B, 2017, 95, .	3.2	19
71	Generation of Anisotropic Massless Dirac Fermions and Asymmetric Klein Tunneling in Few-Layer Black Phosphorus Superlattices. Nano Letters, 2017, 17, 2280-2286.	9.1	52
72	High thermoelectric power factor in two-dimensional crystals of $\text{MoS}_2$ . Physical Review B, 2017, 95, .	3.2	201

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73	Discovery of intrinsic ferromagnetism in two-dimensional van der Waals crystals. <i>Nature</i> , 2017, 546, 265-269.	27.8	3,260
74	Anomalous Anderson localization behaviors in disordered pseudospin systems. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 4087-4092.	7.1	27
75	Atomically precise graphene nanoribbon heterojunctions from a single molecular precursor. <i>Nature Nanotechnology</i> , 2017, 12, 1077-1082.	31.5	162
76	Dynamics of Symmetry-Breaking Stacking Boundaries in Bilayer MoS <sub>2</sub> . <i>Journal of Physical Chemistry C</i> , 2017, 121, 22559-22566.	3.1	22
77	Topological Phases in Graphene Nanoribbons: Junction States, Spin Centers, and Quantum Spin Chains. <i>Physical Review Letters</i> , 2017, 119, 076401.	7.8	235
78	Tunable excitons in bilayer graphene. <i>Science</i> , 2017, 358, 907-910.	12.6	126
79	Magnetic brightening and control of dark excitons in monolayer WSe <sub>2</sub> . <i>Nature Nanotechnology</i> , 2017, 12, 883-888.	31.5	315
80	Symmetry rules shaping spin-orbital textures in surface states. <i>Physical Review B</i> , 2017, 95, .	3.2	9
81	Environmental Screening Effects in 2D Materials: Renormalization of the Bandgap, Electronic Structure, and Optical Spectra of Few-Layer Black Phosphorus. <i>Nano Letters</i> , 2017, 17, 4706-4712.	9.1	155
82	Direct observation of the layer-dependent electronic structure in phosphorene. <i>Nature Nanotechnology</i> , 2017, 12, 21-25.	31.5	625
83	Origins of Singlet Fission in Solid Pentacene from an <i>ab initio</i> Green's Function Approach. <i>Physical Review Letters</i> , 2017, 119, 267401.	7.8	55
84	Quasiparticle energies and dielectric functions of diamond polytypes. <i>Physical Review Materials</i> , 2017, 1, .	2.4	5
85	Real-space study of the optical absorption in alternative phases of silicon. <i>Physical Review Materials</i> , 2017, 1, .	2.4	2
86	Low rank approximation in G <sub>0</sub> W <sub>0</sub> calculations. <i>Science China Mathematics</i> , 2016, 59, 1593-1612.	1.7	14
87	Temperature-Induced Topological Phase Transitions: Promoted versus Suppressed Nontrivial Topology. <i>Physical Review Letters</i> , 2016, 117, 246401.	7.8	39
88	Excitation spectra of aromatic molecules within a real-space $G_0W_0$ formalism: Role of self-consistency and vertex corrections. <i>Physical Review B</i> , 2016, 94, .	3.2	58
89	Automated construction of maximally localized Wannier functions for bands with nontrivial topology. <i>Physical Review B</i> , 2016, 94, .	3.2	4
90	Formation and Dynamics of Electron-Irradiation-Induced Defects in Hexagonal Boron Nitride at Elevated Temperatures. <i>Nano Letters</i> , 2016, 16, 7142-7147.	9.1	49

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91	Electrostatically Driven Nanoballoon Actuator. Nano Letters, 2016, 16, 6787-6791.	9.1	16
92	Ab initioelectronic relaxation times and transport in noble metals. Physical Review B, 2016, 94, .	3.2	56
93	Gate Switchable Transport and Optical Anisotropy in 90° Twisted Bilayer Black Phosphorus. Nano Letters, 2016, 16, 5542-5546.	9.1	71
94	Tuning charge and correlation effects for a single molecule on a graphene device. Nature Communications, 2016, 7, 13553.	12.8	82
95	Dispersion and line shape of plasmon satellites in one, two, and three dimensions. Physical Review B, 2016, 93, .	3.2	15
96	Klein tunneling and supercollimation of pseudospin-1 electromagnetic waves. Physical Review B, 2016, 93, .	3.2	93
97	Spectral functions of the uniform electron gas via coupled-cluster theory and comparison to the related approximations. Physical Review B, 2016, 93, .	3.2	70
98	Screening and many-body effects in two-dimensional crystals: Monolayer MoS <sub>2</sub> . Physical Review B, 2016, 93, .	3.2	298
99	Proposal for a bulk material based on a monolayer FeSe on SrTiO <sub>3</sub> superconductor. Physical Review B, 2016, 93, .	3.2	16
100	Effective mass in bilayer graphene at low carrier densities: The role of potential disorder and electron-electron interaction. Physical Review B, 2016, 94, .	3.2	16
101	Bottom-Up Synthesis of $N = 13$ Sulfur-Doped Graphene Nanoribbons. Journal of Physical Chemistry C, 2016, 120, 2684-2687.	3.1	119
102	SU(4) symmetry breaking revealed by magneto-optical spectroscopy in epitaxial graphene. Physical Review B, 2015, 91, .	3.2	2
103	Automated construction of maximally localized Wannier functions: Optimized projection functions method. Physical Review B, 2015, 92, .	3.2	33
104	Theory and computation of hot carriers generated by surface plasmon polaritons in noble metals. Nature Communications, 2015, 6, 7044.	12.8	317
105	Nonanalyticity, Valley Quantum Phases, and Lightlike Exciton Dispersion in Monolayer Transition Metal Dichalcogenides: Theory and First-Principles Calculations. Physical Review Letters, 2015, 115, 176801.	7.8	196
106	Numerical integration for ab initio many-electron self energy calculations within the GW approximation. Journal of Computational Physics, 2015, 286, 1-13.	3.8	15
107	First-principles theory of electron-spin fluctuation coupling and superconducting instabilities in iron selenide. Physical Review B, 2015, 91, .	3.2	13
108	Molecular bandgap engineering of bottom-up synthesized graphene nanoribbon heterojunctions. Nature Nanotechnology, 2015, 10, 156-160.	31.5	414







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127	Probing excitonic dark states in single-layer tungsten disulphide. Nature, 2014, 513, 214-218.	27.8	835
128	Giant bandgap renormalization and excitonic effects in a monolayer transition metal dichalcogenide semiconductor. Nature Materials, 2014, 13, 1091-1095.	27.5	1,470
129	<i>Ab Initio</i> Study of Hot Carriers in the First Picosecond after Sunlight Absorption in Silicon. Physical Review Letters, 2014, 112, 257402.	7.8	203
130	Electron Supercollimation in Graphene and Dirac Fermion Materials Using One-Dimensional Disorder Potentials. Physical Review Letters, 2014, 113, 026802.	7.8	24
131	Imaging and Tuning Molecular Levels at the Surface of a Gated Graphene Device. ACS Nano, 2014, 8, 5395-5401.	14.6	39
132	Tuning Many-Body Interactions in Graphene: The Effects of Doping on Excitons and Carrier Lifetimes. Physical Review Letters, 2014, 112, .	7.8	74
133	Band offsets in c-Si/Si-XII heterojunctions. Solid State Communications, 2014, 191, 6-9.	1.9	0
134	Optical Spectrum of $\text{MoS}_2$ Many-Body Effects and Diversity of Exciton States. Physical Review Letters, 2013, 111, 216805.	7.8	1,275
135	Photoelectron spin-flipping and texture manipulation in a topological insulator. Nature Physics, 2013, 9, 293-298.	16.7	176
136	Observing Atomic Collapse Resonances in Artificial Nuclei on Graphene. Science, 2013, 340, 734-737.	12.6	223
137	Physical Origin of Satellites in Photoemission of Doped Graphene: An <i>Ab Initio</i> GW Plus Cumulant Study. Physical Review Letters, 2013, 110, 146801.	7.8	97
138	Coulomb-hole summations and energies for $G$ and $W$ calculations with limited number of empty orbitals: A modified static remainder approach. Physical Review B, 2013, 87, .	3.2	149
139	Intermolecular interactions and substrate effects for an adamantane monolayer on a Au(111) surface. Physical Review B, 2013, 88, .	3.2	6
140	Tuning two-dimensional band structure of Cu(111) surface-state electrons that interplay with artificial supramolecular architectures. Physical Review B, 2013, 88, .	3.2	42
141	Resonant Excitation of Graphene K-Phonon and Intra-Landau-Level Excitons in Magneto-Optical Spectroscopy. Physical Review Letters, 2012, 108, 247401.	7.8	11
142	Phonon-Assisted Optical Absorption in Silicon from First Principles. Physical Review Letters, 2012, 108, 167402.	7.8	143
143	Anomalous insulator-metal transition in boron nitride-graphene hybrid atomic layers. Physical Review B, 2012, 86, .	3.2	42
144	Spin Polarization of Photoelectrons from Topological Insulators. Physical Review Letters, 2012, 109, 097601.	7.8	89



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163	EPW: A program for calculating the electron-phonon coupling using maximally localized Wannier functions. Computer Physics Communications, 2010, 181, 2140-2148.	7.5	324
164	Ab initio calculations of pressure-induced structural phase transitions of GeTe. Physical Review B, 2010, 82, .	3.2	27
165	Quasiparticle electronic structure of bismuth telluride in the $GW$ approximation. Physical Review B, 2010, 82, .	3.2	59
166	Selective functionalization of halogens on zigzag graphene nanoribbons: A route to the separation of zigzag graphene nanoribbons. Applied Physics Letters, 2010, 97, 233101.	3.3	23
167	Tunable Excitons in Biased Bilayer Graphene. Nano Letters, 2010, 10, 426-431.	9.1	81
168	Spin Polarization and Transport of Surface States in the Topological Insulators $Bi_2Se_3$ and $Bi_2Te_3$ . Physical Review Letters, 2010, 105, 266806.	7.8	424
169	GW method with the self-consistent Sternheimer equation. Physical Review B, 2010, 81, .	3.2	122
170	Electronic and optical properties of body-centered-tetragonal Si and Ge. Physical Review B, 2010, 81, .	3.2	29
171	Electron-phonon coupling in $C_{60}$ hybrid functionals. Physical Review B, 2010, 81, .	3.2	43
172	Quasiparticle Band Gap of ZnO: High Accuracy from the Conventional $GW_0$ . Physical Review Letters, 2010, 105, 146401.	7.8	212
173	Electron-Phonon Renormalization of the Direct Band Gap of Diamond. Physical Review Letters, 2010, 105, 265501.	7.8	241
174	Calcium-Decorated Graphene-Based Nanostructures for Hydrogen Storage. Nano Letters, 2010, 10, 793-798.	9.1	331
175	Graphene Dirac fermions in one-dimensional inhomogeneous field profiles: Transforming magnetic to electric field. Physical Review B, 2010, 81, .	3.2	98
176	Prediction of superconducting properties of $CaB_2$ anisotropic Eliashberg theory. Physical Review B, 2009, 80, .	3.2	35
177	Angle-Resolved Photoemission Spectra of Graphene from First-Principles Calculations. Nano Letters, 2009, 9, 4234-4239.	9.1	102
178	Mechanically controlled binary conductance switching of a single-molecule junction. Nature Nanotechnology, 2009, 4, 230-234.	31.5	609
179	Electron-Hole Interaction in Carbon Nanotubes: Novel Screening and Exciton Excitation Spectra. Nano Letters, 2009, 9, 1330-1334.	9.1	64
180	Calcium-decorated carbon nanotubes for high-capacity hydrogen storage: First-principles calculations. Physical Review B, 2009, 80, .	3.2	148

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181	First-Principles Study of Electron Linewidths in Graphene. Physical Review Letters, 2009, 102, 076803.	7.8	72
182	Excitonic Effects on the Optical Response of Graphene and Bilayer Graphene. Physical Review Letters, 2009, 103, 186802.	7.8	604
183	Landau Levels and Quantum Hall Effect in Graphene Superlattices. Physical Review Letters, 2009, 103, 046808.	7.8	137
184	Making Massless Dirac Fermions from a Patterned Two-Dimensional Electron Gas. Nano Letters, 2009, 9, 1793-1797.	9.1	151
185	Anisotropic Eliashberg theory for superconductivity in compressed and doped $MgB_2$ . Physical Review B, 2009, 79, .	3.2	17
186	GW approach to Anderson model out of equilibrium: Coulomb blockade and false hysteresis in the $\nu$ characteristics. Physical Review B, 2009, 79, .	3.2	51
187	Small phonon contribution to the photoemission kink in the copper oxide superconductors. Nature, 2008, 452, 975-978.	27.8	157
188	Anisotropic behaviours of massless Dirac fermions in graphene under periodic potentials. Nature Physics, 2008, 4, 213-217.	16.7	609
189	Electron Beam Supercollimation in Graphene Superlattices. Nano Letters, 2008, 8, 2920-2924.	9.1	253
190	Optimization of metal dispersion in doped graphitic materials for hydrogen storage. Physical Review B, 2008, 78, .	3.2	111
191	quasiparticle corrections to the structure of bcc hydrogen. Physical Review B, 2008, 77, .	3.2	34
192	Electron-Phonon Interactions in Graphene, Bilayer Graphene, and Graphite. Nano Letters, 2008, 8, 4229-4233.	9.1	156
193	New Generation of Massless Dirac Fermions in Graphene under External Periodic Potentials. Physical Review Letters, 2008, 101, 126804.	7.8	370
194	Negative Differential Resistance in Carbon Atomic Wire-Carbon Nanotube Junctions. Nano Letters, 2008, 8, 2900-2905.	9.1	160
195	Van Hove singularity and apparent anisotropy in the electron-phonon interaction in graphene. Physical Review B, 2008, 77, .	3.2	50
196	Contact dependence of the conductance of molecular junctions from first principles. Physical Review B, 2008, 77, .	3.2	12
197	Low-energy structures of K atoms in expanded $K_3C_{60}$ monolayers: Ab initio pseudopotential density-functional calculations. Physical Review B, 2008, 77, .	3.2	3
198	Electron-phonon interaction using Wannier functions. Physical Review B, 2007, 76, .	3.2	625

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199	Velocity Renormalization and Carrier Lifetime in Graphene from the Electron-Phonon Interaction. <i>Physical Review Letters</i> , 2007, 99, 086804.	7.8	183
200	Negative Differential Resistance in Transport through Organic Molecules on Silicon. <i>Physical Review Letters</i> , 2007, 98, 066807.	7.8	54
201	First-principles scattering-state approach for nonlinear electrical transport in nanostructures. <i>Physical Review B</i> , 2007, 76, .	3.2	53
202	Electronic Structure and Energetics of MgB <sub>2</sub> Nanotube. <i>Journal of the Physical Society of Japan</i> , 2007, 76, 043707.	1.6	7
203	Quasiparticle Energies and Band Gaps in Graphene Nanoribbons. <i>Physical Review Letters</i> , 2007, 99, 186801.	7.8	1,092
204	Enhanced electron-hole interaction and optical absorption in a silicon nanowire. <i>Physical Review B</i> , 2007, 75, .	3.2	65
205	Amine-Linked Gold Linked Single-Molecule Circuits: Experiment and Theory. <i>Nano Letters</i> , 2007, 7, 3477-3482.	9.1	447
206	Bound Excitons in Metallic Single-Walled Carbon Nanotubes. <i>Nano Letters</i> , 2007, 7, 1626-1630.	9.1	105
207	Excitonic Effects in the Optical Spectra of Graphene Nanoribbons. <i>Nano Letters</i> , 2007, 7, 3112-3115.	9.1	254
208	Vibrational properties of single walled carbon nanotubes under pressure from Raman scattering experiments and molecular dynamics simulations. <i>Physica Status Solidi (B): Basic Research</i> , 2007, 244, 121-126.	1.5	11
209	Excitons in carbon nanotubes: Diameter and chirality trends. <i>Physica Status Solidi (B): Basic Research</i> , 2007, 244, 4016-4020.	1.5	35
210	Hypothetical hard structures of carbon with cubic symmetry. <i>Physical Review B</i> , 2006, 74, .	3.2	66
211	Quasiparticle energy of semicore electrons in ZnS: Combined LDA+U and GW approach. <i>Physical Review B</i> , 2006, 74, .	3.2	65
212	Renormalization of Molecular Electronic Levels at Metal-Molecule Interfaces. <i>Physical Review Letters</i> , 2006, 97, 216405.	7.8	769
213	First-principles studies of the electronic structure of cyclopentene on Si(001): density functional theory and GW calculations. <i>Physica Status Solidi (B): Basic Research</i> , 2006, 243, 2048-2053.	1.5	12
214	First direct observation of Dirac fermions in Graphite. <i>Nature Physics</i> , 2006, 2, 595-599.	16.7	466
215	Half-metallic graphene nanoribbons. <i>Nature</i> , 2006, 444, 347-349.	27.8	3,878
216	Diameter and chirality dependence of exciton properties in carbon nanotubes. <i>Physical Review B</i> , 2006, 74, .	3.2	179

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217	Selection rules for one- and two-photon absorption by excitons in carbon nanotubes. Physical Review B, 2006, 73, .	3.2	48
218	Energy Gaps in Graphene Nanoribbons. Physical Review Letters, 2006, 97, 216803.	7.8	4,396
219	Spectroscopy of zigzag single-walled carbon nanotubes: Comparing femtosecond transient absorption spectra with ab initio calculations. Physical Review B, 2006, 74, .	3.2	29
220	Anisotropic Eliashberg theory and the two-band model for the superconducting properties of MgB <sub>2</sub> . Physical Review B, 2006, 73, .	3.2	27
221	Electron transport and optical properties of carbon nanostructures from first principles. Computer Physics Communications, 2005, 169, 1-8.	7.5	16
222	Temperature and Hydrostatic Pressure Effects on the Band Gap of Semiconducting Carbon Nanotubes. AIP Conference Proceedings, 2005, , .	0.4	0
223	Excitonic Effects and Optical Spectra of Single-Walled Carbon Nanotubes. AIP Conference Proceedings, 2005, , .	0.4	6
224	Family Behavior of the Pressure and Temperature Dependences of the Band Gap of Semiconducting Carbon Nanotubes. AIP Conference Proceedings, 2005, , .	0.4	0
225	Spatially Dependent Inelastic Tunneling in Gd@C <sub>82</sub> . AIP Conference Proceedings, 2005, , .	0.4	0
226	Coexistence of sharp quasiparticle dispersions and disorder features in graphite. Physical Review B, 2005, 71, .	3.2	59
227	Mechanism for bias-assisted indium mass transport on carbon nanotube surfaces. Physical Review B, 2005, 72, .	3.2	22
228	Structural and electronic properties of carbon in hybrid diamond-graphite structures. Physical Review B, 2005, 72, .	3.2	77
229	Temperature Dependence of the Band Gap of Semiconducting Carbon Nanotubes. Physical Review Letters, 2005, 94, 036801.	7.8	119
230	Theory of sodium ordering in Na <sub>x</sub> CoO <sub>2</sub> . Physical Review B, 2005, 71, .	3.2	102
231	Theory and Ab Initio Calculation of Radiative Lifetime of Excitons in Semiconducting Carbon Nanotubes. Physical Review Letters, 2005, 95, 247402.	7.8	295
232	Reply to "Comment on 'First-principles calculation of the superconducting transition in MgB <sub>2</sub> within the anisotropic Eliashberg formalism'" Physical Review B, 2004, 69, .	3.2	19
233	Ab initio calculation of band-gap renormalization in highly excited GaAs. Physical Review B, 2004, 69, .	3.2	45
234	Excitonic Effects and Optical Spectra of Single-Walled Carbon Nanotubes. Physical Review Letters, 2004, 92, 077402.	7.8	875

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