Steven G Louie

List of Publications by Citations

286 papers	48,919 citations	96 h-index	220 g-index
304 ext. papers	54,855 ext. citations	9.8 avg, IF	7.78 L-index

#	Paper	IF	Citations
286	Energy gaps in graphene nanoribbons. *Physical Review Letters*, **2006**, 97, 216803	7.4	3863
285	Half-metallic graphene nanoribbons. *Nature*, **2006**, 444, 347-9	50.4	3486
284	Electron correlation in semiconductors and insulators: Band gaps and quasiparticle energies. *Physical Review B*, **1986**, 34, 5390-5413	3.3	2875
283	Relaxation of Crystals with the Quasi-Newton Method. *Journal of Computational Physics*, **1997**, 131, 233-240	4.1	1913
282	Discovery of intrinsic ferromagnetism in two-dimensional van der Waals crystals. *Nature*, **2017**, 546, 265-269	36.4	1890
281	Recent Advances in Two-Dimensional Materials beyond Graphene. *ACS Nano*, **2015**, 9, 11509-39	16.7	1581
280	Electron-hole excitations and optical spectra from first principles. *Physical Review B*, **2000**, 62, 4927-4944	3.3	1151
279	Giant bandgap renormalization and excitonic effects in a monolayer transition metal dichalcogenide semiconductor. *Nature Materials*, **2014**, 13, 1091-5	27	1150
278	First-principles theory of quasiparticles: Calculation of band gaps in semiconductors and insulators. *Physical Review Letters*, **1985**, 55, 1418-1421	7.4	1096
277	Crossed nanotube junctions. *Science*, **2000**, 288, 494-7	33.3	1050
276	Optical spectrum of MoS2: many-body effects and diversity of exciton states. *Physical Review Letters*, **2013**, 111, 216805	7.4	1031
275	Quasiparticle energies and band gaps in graphene nanoribbons. *Physical Review Letters*, **2007**, 99, 186801	7.4	937
274	Excitonic effects and optical spectra of single-walled carbon nanotubes. *Physical Review Letters*, **2004**, 92, 077402	7.4	805
273	Renormalization of molecular electronic levels at metal-molecule interfaces. *Physical Review Letters* , **2006**, 97, 216405	7.4	693
272	Probing excitonic dark states in single-layer tungsten disulphide. *Nature*, **2014**, 513, 214-8	50.4	672
271	Electron-Hole Excitations in Semiconductors and Insulators. *Physical Review Letters*, **1998**, 81, 2312-2315	7.4	600
270	Topological defects in graphene: Dislocations and grain boundaries. *Physical Review B*, **2010**, 81,	3.3	571

269	Spatially resolving edge states of chiral graphene nanoribbons. *Nature Physics*, **2011**, 7, 616-620	16.2	557
268	Electronic mechanism of hardness enhancement in transition-metal carbonitrides. *Nature*, **1999**, 399, 132-134	50.4	556
267	Anisotropic behaviours of massless Dirac fermions in graphene under periodic potentials. *Nature Physics*, **2008**, 4, 213-217	16.2	531
266	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	4.3	530
265	Mechanically controlled binary conductance switching of a single-molecule junction. *Nature Nanotechnology*, **2009**, 4, 230-4	28.7	515
264	Excitonic effects on the optical response of graphene and bilayer graphene. *Physical Review Letters*, **2009**, 103, 186802	7.4	509
263	Direct observation of the layer-dependent electronic structure in phosphorene. *Nature Nanotechnology*, **2017**, 12, 21-25	28.7	473
262	First direct observation of Dirac fermions in graphite. *Nature Physics*, **2006**, 2, 595-599	16.2	430
261	Electron-phonon interaction using Wannier functions. *Physical Review B*, **2007**, 76,	3.3	425
260	Fully collapsed carbon nanotubes. *Nature*, **1995**, 377, 135-138	50.4	419
259	Amine-gold linked single-molecule circuits: experiment and theory. *Nano Letters*, **2007**, 7, 3477-82	11.5	403
258	Spin polarization and transport of surface states in the topological insulators Bi2Se3 and Bi2Te3 from first principles. *Physical Review Letters*, **2010**, 105, 266806	7.4	381
257	Disorder, Pseudospins, and Backscattering in Carbon Nanotubes. *Physical Review Letters*, **1999**, 83, 5098-5101	7.4	371
256	Molecular bandgap engineering of bottom-up synthesized graphene nanoribbon heterojunctions. *Nature Nanotechnology*, **2015**, 10, 156-60	28.7	340
255	New generation of massless Dirac fermions in graphene under external periodic potentials. *Physical Review Letters*, **2008**, 101, 126804	7.4	316
254	Broken symmetry and pseudogaps in ropes of carbon nanotubes. *Nature*, **1998**, 391, 466-468	50.4	312
253	Ab initio static dielectric matrices from the density-functional approach. I. Formulation and application to semiconductors and insulators. *Physical Review B*, **1987**, 35, 5585-5601	3.3	311
252	Excitonic Effects and the Optical Absorption Spectrum of Hydrogenated Si Clusters. *Physical Review Letters*, **1998**, 80, 3320-3323	7.4	310

251	Calcium-decorated graphene-based nanostructures for hydrogen storage. *Nano Letters*, **2010**, 10, 793-8	11.5	300
250	First-principles calculation of the superconducting transition in MgB2 within the anisotropic Eliashberg formalism. *Physical Review B*, **2002**, 66,	3.3	295
249	Topological band engineering of graphene nanoribbons. *Nature*, **2018**, 560, 204-208	50.4	287
248	Tunable Magnetism and Half-Metallicity in Hole-Doped Monolayer GaSe. *Physical Review Letters*, **2015**, 114, 236602	7.4	257
247	Ab initio calculation of the electronic and optical properties of solid pentacene. *Physical Review B*, **2003**, 67,	3.3	252
246	Vacancy hardening and softening in transition metal carbides and nitrides. *Physical Review Letters*, **2001**, 86, 3348-51	7.4	251
245	Theory and ab initio calculation of radiative lifetime of excitons in semiconducting carbon nanotubes. *Physical Review Letters*, **2005**, 95, 247402	7.4	248
244	Theory and computation of hot carriers generated by surface plasmon polaritons in noble metals. *Nature Communications*, **2015**, 6, 7044	17.4	238
243	EPW: A program for calculating the electron–phonon coupling using maximally localized Wannier functions. *Computer Physics Communications*, **2010**, 181, 2140-2148	4.2	225
242	Excitonic effects in the optical spectra of graphene nanoribbons. *Nano Letters*, **2007**, 7, 3112-5	11.5	225
241	Electron beam supercollimation in graphene superlattices. *Nano Letters*, **2008**, 8, 2920-4	11.5	223
240	Screening and many-body effects in two-dimensional crystals: Monolayer MoS2. *Physical Review B*, **2016**, 93,	3.3	217
239	Magnetic brightening and control of dark excitons in monolayer WSe. *Nature Nanotechnology*, **2017**, 12, 883-888	28.7	213
238	GW100: Benchmarking G0W0 for Molecular Systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 5665-87	6.4	207
237	Gate-controlled ionization and screening of cobalt adatoms on a graphene surface. *Nature Physics*, **2011**, 7, 43-47	16.2	198
236	Electron-phonon renormalization of the direct band gap of diamond. *Physical Review Letters*, **2010**, 105, 265501	7.4	192
235	Quasiparticle band gap of ZnO: high accuracy from the conventional G₀W₀ approach. *Physical Review Letters*, **2010**, 105, 146401	7.4	180
234	Excitons and Optical Spectrum of the Si(111)(2×1) Surface. *Physical Review Letters*, **1999**, 83, 856-859	7.4	178

233	Site-Specific Substitutional Boron Doping of Semiconducting Armchair Graphene Nanoribbons. *Journal of the American Chemical Society*, **2015**, 137, 8872-5	16.4	177
232	Observing atomic collapse resonances in artificial nuclei on graphene. *Science*, **2013**, 340, 734-7	33.3	175
231	Diameter and chirality dependence of exciton properties in carbon nanotubes. *Physical Review B*, **2006**, 74,	3.3	168
230	ab initio study of hot carriers in the first picosecond after sunlight absorption in silicon. *Physical Review Letters*, **2014**, 112, 257402	7.4	166
229	Many-body interactions in quasi-freestanding graphene. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 11365-9	11.5	166
228	Velocity renormalization and carrier lifetime in graphene from the electron-phonon interaction. *Physical Review Letters*, **2007**, 99, 086804	7.4	162
227	High accuracy many-body calculational approaches for excitations in molecules. *Physical Review Letters*, **2001**, 86, 472-5	7.4	160
226	Ab Initio Photoabsorption Spectra and Structures of Small Semiconductor and Metal Clusters. *Physical Review Letters*, **1996**, 77, 247-250	7.4	156
225	Photoelectron spin-flipping and texture manipulation in a topological insulator. *Nature Physics*, **2013**, 9, 293-298	16.2	152
224	Negative differential resistance in carbon atomic wire-carbon nanotube junctions. *Nano Letters*, **2008**, 8, 2900-5	11.5	152
223	Topological Phases in Graphene Nanoribbons: Junction States, Spin Centers, and Quantum Spin Chains. *Physical Review Letters*, **2017**, 119, 076401	7.4	151
222	Structural forms of cubic BC2N. *Physical Review B*, **2001**, 64,	3.3	146
221	Si-O-Si bond-angle distribution in vitreous silica from first-principles 29Si NMR analysis. *Physical Review B*, **2000**, 62, R4786-R4789	3.3	145
220	Self-consistent pseudopotential method for localized configurations: Molecules. *Physical Review B*, **1975**, 12, 5575-5579	3.3	145
219	Electron-phonon interactions in graphene, bilayer graphene, and graphite. *Nano Letters*, **2008**, 8, 4229-33	11.5	138
218	Three-dimensional spirals of atomic layered MoS2. *Nano Letters*, **2014**, 14, 6418-23	11.5	136
217	Calcium-decorated carbon nanotubes for high-capacity hydrogen storage: First-principles calculations. *Physical Review B*, **2009**, 80,	3.3	135
216	Small phonon contribution to the photoemission kink in the copper oxide superconductors. *Nature*, **2008**, 452, 975-8	50.4	135

215	High thermoelectric power factor in two-dimensional crystals of MoS2. *Physical Review B*, **2017**, 95,	3.3	133
214	Nonanalyticity, Valley Quantum Phases, and Lightlike Exciton Dispersion in Monolayer Transition Metal Dichalcogenides: Theory and First-Principles Calculations. *Physical Review Letters*, **2015**, 115, 176801	7.4	130
213	Landau levels and quantum Hall effect in graphene superlattices. *Physical Review Letters*, **2009**, 103, 046808	7.4	125
212	Inversion symmetry and bulk Rashba effect in methylammonium lead iodide perovskite single crystals. *Nature Communications*, **2018**, 9, 1829	17.4	123
211	Low Energy Properties of (n,n) Carbon Nanotubes. *Physical Review Letters*, **1997**, 78, 4245-4248	7.4	123
210	Making massless Dirac fermions from a patterned two-dimensional electron gas. *Nano Letters*, **2009**, 9, 1793-7	11.5	120
209	Coulomb-hole summations and energies for GW calculations with limited number of empty orbitals: A modified static remainder approach. *Physical Review B*, **2013**, 87,	3.3	119
208	Atomically precise graphene nanoribbon heterojunctions from a single molecular precursor. *Nature Nanotechnology*, **2017**, 12, 1077-1082	28.7	118
207	Structural and electronic properties of n-doped and p-doped SrTiO3. *Physical Review B*, **2004**, 70,	3.3	118
206	Identifying substitutional oxygen as a prolific point defect in monolayer transition metal dichalcogenides. *Nature Communications*, **2019**, 10, 3382	17.4	117
205	Mechanical instability and ideal shear strength of transition metal carbides and nitrides. *Physical Review Letters*, **2001**, 87, 075503	7.4	111
204	Probing the role of interlayer coupling and coulomb interactions on electronic structure in few-layer MoSe□nanostructures. *Nano Letters*, **2015**, 15, 2594-9	11.5	110
203	Phonon-assisted optical absorption in silicon from first principles. *Physical Review Letters*, **2012**, 108, 167402	7.4	110
202	Self-Consistent Pseudopotential Calculations on Si(111) Unreconstructed and (2□) Reconstructed Surfaces. *Physical Review Letters*, **1975**, 34, 1385-1388	7.4	109
201	Excitonic effects in the optical properties of a SiC sheet and nanotubes. *Physical Review B*, **2011**, 84,	3.3	108
200	Self-Consistent Pseudopotential Calculation for a Metal-Semiconductor Interface. *Physical Review Letters*, **1975**, 35, 866-869	7.4	107
199	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	11.5	105
198	Optimization of metal dispersion in doped graphitic materials for hydrogen storage. *Physical Review B*, **2008**, 78,	3.3	105

197	Temperature dependence of the band gap of semiconducting carbon nanotubes. *Physical Review Letters*, **2005**, 94, 036801	7.4	105
196	NMR Chemical Shifts of Ice and Liquid Water:´The Effects of Condensation. *Journal of the American Chemical Society*, **2000**, 122, 123-129	16.4	102
195	Quasiparticle effects in the bulk and surface-state bands of Bi2Se3 and Bi2Te3 topological insulators. *Physical Review B*, **2012**, 85,	3.3	101
194	Computational design of direct-bandgap semiconductors that lattice-match silicon. *Nature*, **2001**, 409, 69-71	50.4	99
193	GW method with the self-consistent Sternheimer equation. *Physical Review B*, **2010**, 81,	3.3	98
192	Theory of sodium ordering in NaxCoO2. *Physical Review B*, **2005**, 71,	3.3	98
191	Theory of magnetic edge states in chiral graphene nanoribbons. *Physical Review B*, **2011**, 84,	3.3	96
190	Observation of carrier-density-dependent many-body effects in graphene via tunneling spectroscopy. *Physical Review Letters*, **2010**, 104, 036805	7.4	96
189	Structural deformation and intertube conductance of crossed carbon nanotube junctions. *Physical Review Letters*, **2001**, 86, 688-91	7.4	96
188	Quasiparticle excitation spectrum for nearly-free-electron metals. *Physical Review B*, **1989**, 39, 8198-8208	3.3	96
187	Fundamentals of Condensed Matter Physics **2016**,		96
186	Bottom-Up Synthesis of N = 13 Sulfur-Doped Graphene Nanoribbons. *Journal of Physical Chemistry C*, **2016**, 120, 2684-2687	3.8	95
185	Angle-resolved photoemission spectra of graphene from first-principles calculations. *Nano Letters*, **2009**, 9, 4234-9	11.5	93
184	Bound excitons in metallic single-walled carbon nanotubes. *Nano Letters*, **2007**, 7, 1626-30	11.5	93
183	Ab initio study of hot electrons in GaAs. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 5291-6	11.5	92
182	Quasiparticle band structure of ZnS and ZnSe. *Physical Review B*, **2002**, 66,	3.3	92
181	Ab initio study of silicon in the R8 phase. *Physical Review B*, **1997**, 56, 6662-6668	3.3	91
180	Tunable excitons in bilayer graphene. *Science*, **2017**, 358, 907-910	33.3	89

179	Spin polarization of photoelectrons from topological insulators. *Physical Review Letters*, **2012**, 109, 097601	7.4	82
178	Physical origin of satellites in photoemission of doped graphene: an ab initio GW plus cumulant study. *Physical Review Letters*, **2013**, 110, 146801	7.4	82
177	Hydrostatic pressure effects on the structural and electronic properties of carbon nanotubes. *Physica Status Solidi (B): Basic Research*, **2004**, 241, 3352-3359	1.3	82
176	Excitons and optical properties of alpha-quartz. *Physical Review Letters*, **2000**, 85, 2613-6	7.4	81
175	Graphene Dirac fermions in one-dimensional inhomogeneous field profiles: Transforming magnetic to electric field. *Physical Review B*, **2010**, 81,	3.3	80
174	Large Spin-Orbit Splitting of Deep In-Gap Defect States of Engineered Sulfur Vacancies in Monolayer WS_{2}. *Physical Review Letters*, **2019**, 123, 076801	7.4	75
173	First-principles DFT+GW study of oxygen vacancies in rutile TiO2. *Physical Review B*, **2014**, 89,	3.3	75
172	Structural and electronic properties of carbon in hybrid diamond-graphite structures. *Physical Review B*, **2005**, 72,	3.3	75
171	Doping effects on the electronic and structural properties of CoO2: An LSDA+U study. *Physical Review B*, **2004**, 70,	3.3	73
170	Theory of semiconductor surface states and metal□semiconductor interfaces. *Journal of Vacuum Science and Technology*, **1976**, 13, 790-797		71
169	Defect-Induced Modification of Low-Lying Excitons and Valley Selectivity in Monolayer Transition Metal Dichalcogenides. *Physical Review Letters*, **2018**, 121, 167402	7.4	69
168	Tuning charge and correlation effects for a single molecule on a graphene device. *Nature Communications*, **2016**, 7, 13553	17.4	66
167	Tunable excitons in biased bilayer graphene. *Nano Letters*, **2010**, 10, 426-31	11.5	66
166	First-principles study of electron linewidths in graphene. *Physical Review Letters*, **2009**, 102, 076803	7.4	65
165	Direct measurement of quantum phases in graphene via photoemission spectroscopy. *Physical Review B*, **2011**, 84,	3.3	64
164	Klein tunneling and supercollimation of pseudospin-1 electromagnetic waves. *Physical Review B*, **2016**, 93,	3.3	62
163	Spectral functions of the uniform electron gas via coupled-cluster theory and comparison to the GW and related approximations. *Physical Review B*, **2016**, 93,	3.3	62
162	Large electron□phonon interactions from FeSe phonons in a monolayer. *New Journal of Physics*, **2015**, 17, 073027	2.9	61

161	Ab initio NMR Chemical Shift of Diamond, Chemical-Vapor-Deposited Diamond, and Amorphous Carbon. *Physical Review Letters*, **1997**, 79, 2340-2343	7.4	61
160	NMR Chemical Shifts in Hard Carbon Nitride Compounds. *Physical Review Letters*, **1998**, 80, 3388-3391	7.4	61
159	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, 7564-9	11.5	59
158	Quasiparticle energy of semicore d electrons in ZnS: Combined LDA+U and GW approach. *Physical Review B*, **2006**, 74,	3.3	59
157	Anomalous quasiparticle lifetime in graphite: band structure effects. *Physical Review Letters*, **2001**, 87, 246405	7.4	59
156	Phonon Softening and Superconductivity in Tellurium under Pressure. *Physical Review Letters*, **1996** , 77, 1151-1154	7.4	59
155	Evaluation of quasiparticle energies for semiconductors without inversion symmetry. *Physical Review B*, **1989**, 40, 3162-3168	3.3	58
154	Tuning Many-Body Interactions in Graphene: The Effects of Doping on Excitons and Carrier Lifetimes. *Physical Review Letters*, **2014**, 112,	7.4	57
153	Electron-hole interaction in carbon nanotubes: novel screening and exciton excitation spectra. *Nano Letters*, **2009**, 9, 1330-4	11.5	57
152	Enhanced electron-hole interaction and optical absorption in a silicon nanowire. *Physical Review B*, **2007**, 75,	3.3	57
151	Gate Switchable Transport and Optical Anisotropy in 90° Twisted Bilayer Black Phosphorus. *Nano Letters*, **2016**, 16, 5542-6	11.5	56
150	Coexistence of sharp quasiparticle dispersions and disorder features in graphite. *Physical Review B*, **2005**, 71,	3.3	56
149	Strong correlations and orbital texture in single-layer 1T-TaSe2. *Nature Physics*, **2020**, 16, 218-224	16.2	56
148	Hierarchical On-Surface Synthesis of Graphene Nanoribbon Heterojunctions. *ACS Nano*, **2018**, 12, 2193-2200	13.7	55
147	Hypothetical hard structures of carbon with cubic symmetry. *Physical Review B*, **2006**, 74,	3.3	55
146	A dielectric-defined lateral heterojunction in a monolayer semiconductor. *Nature Electronics*, **2019**, 2, 60-65	28.4	53
145	Ultrasensitive tunability of the direct bandgap of 2D InSe flakes via strain engineering. *2D Materials* , **2018**, 5, 021002	5.9	53
144	Coupling of nonlocal potentials to electromagnetic fields. *Physical Review Letters*, **2001**, 87, 087402	7.4	51

143	Quasiparticle electronic structure of bismuth telluride in the GW approximation. *Physical Review B*, **2010**, 82,	3.3	50
142	Quasiparticle excitations and charge transition levels of oxygen vacancies in hafnia. *Physical Review Letters*, **2011**, 107, 216803	7.4	50
141	Negative differential resistance in transport through organic molecules on silicon. *Physical Review Letters*, **2007**, 98, 066807	7.4	50
140	First-principles scattering-state approach for nonlinear electrical transport in nanostructures. *Physical Review B*, **2007**, 76,	3.3	50
139	GW approach to Anderson model out of equilibrium: Coulomb blockade and false hysteresis in the I V characteristics. *Physical Review B*, **2009**, 79,	3.3	47
138	Nonuniform sampling schemes of the Brillouin zone for many-electron perturbation-theory calculations in reduced dimensionality. *Physical Review B*, **2017**, 95,	3.3	46
137	Van Hove singularity and apparent anisotropy in the electron-phonon interaction in graphene. *Physical Review B*, **2008**, 77,	3.3	46
136	Inducing metallicity in graphene nanoribbons via zero-mode superlattices. *Science*, **2020**, 369, 1597-1603	33.3	46
135	Orbitally Matched Edge-Doping in Graphene Nanoribbons. *Journal of the American Chemical Society* , **2018**, 140, 807-813	16.4	45
134	Ab initio GW quasiparticle calculation of small alkali-metal clusters. *Physical Review B*, **2002**, 65,	3.3	44
133	Selection rules for one- and two-photon absorption by excitons in carbon nanotubes. *Physical Review B*, **2006**, 73,	3.3	43
132	Exchange-driven intravalley mixing of excitons in monolayer transition metal dichalcogenides. *Nature Physics*, **2019**, 15, 228-232	16.2	43
131	Physical origin of giant excitonic and magneto-optical responses in two-dimensional ferromagnetic insulators. *Nature Communications*, **2019**, 10, 2371	17.4	42
130	Molecular Self-Assembly in a Poorly Screened Environment: F4TCNQ on Graphene/BN. *ACS Nano*, **2015**, 9, 12168-73	16.7	42
129	Origins of Singlet Fission in Solid Pentacene from an ab initio Green's Function Approach. *Physical Review Letters*, **2017**, 119, 267401	7.4	42
128	Anomalous insulator-metal transition in boron nitride-graphene hybrid atomic layers. *Physical Review B*, **2012**, 86,	3.3	41
127	Ab initio GW quasiparticle energies of small sodium clusters by an all-electron mixed-basis approach. *Physical Review B*, **2001**, 63,	3.3	41
126	Imaging moir flat bands in three-dimensional reconstructed WSe/WS superlattices. *Nature Materials*, **2021**, 20, 945-950	27	41

125	Ab initio calculation of band-gap renormalization in highly excited GaAs. *Physical Review B*, **2004**, 69,	3.3	40
124	Excitation spectra of aromatic molecules within a real-space GW-BSE formalism: Role of self-consistency and vertex corrections. *Physical Review B*, **2016**, 94,	3.3	40
123	Ab initio electronic relaxation times and transport in noble metals. *Physical Review B*, **2016**, 94,	3.3	40
122	Electron-phonon coupling in C60 using hybrid functionals. *Physical Review B*, **2010**, 81,	3.3	39
121	Formation and Dynamics of Electron-Irradiation-Induced Defects in Hexagonal Boron Nitride at Elevated Temperatures. *Nano Letters*, **2016**, 16, 7142-7147	11.5	39
120	Large enhancement of boron solubility in silicon due to biaxial stress. *Applied Physics Letters*, **2002**, 80, 4738-4740	3.4	38
119	Electromagnetic screening by metals. *American Journal of Physics*, **1988**, 56, 989-992	0.7	38
118	Mechanism for optical initialization of spin in NV□center in diamond. *Physical Review B*, **2012**, 86,	3.3	37
117	Satellite band structure in silicon caused by electron-plasmon coupling. *Physical Review B*, **2015**, 91,	3.3	36
116	Comparing time-dependent density functional theory with many-body perturbation theory for semiconductors: Screened range-separated hybrids and the GW plus Bethe-Salpeter approach. *Physical Review Materials*, **2019**, 3,	3.2	36
115	Electron-Phonon Coupling from Ab´Initio Linear-Response Theory within the GW Method: Correlation-Enhanced Interactions and Superconductivity in Ba_{1-x}K_{x}BiO_{3}. *Physical Review Letters*, **2019**, 122, 186402	7.4	35
114	Tuning two-dimensional band structure of Cu(111) surface-state electrons that interplay with artificial supramolecular architectures. *Physical Review B*, **2013**, 88,	3.3	35
113	Unifying Optical Selection Rules for Excitons in Two Dimensions: Band Topology and Winding Numbers. *Physical Review Letters*, **2018**, 120, 087402	7.4	34
112	Generation of Anisotropic Massless Dirac Fermions and Asymmetric Klein Tunneling in Few-Layer Black Phosphorus Superlattices. *Nano Letters*, **2017**, 17, 2280-2286	11.5	33
111	Imaging and tuning molecular levels at the surface of a gated graphene device. *ACS Nano*, **2014**, 8, 5395-5401	14.7	31
110	Orbital Symmetry and the Optical Response of Single-Layer MX Monochalcogenides. *Nano Letters*, **2018**, 18, 1925-1929	11.5	30
109	Direct observation of Klein tunneling in phononic crystals. *Science*, **2020**, 370, 1447-1450	33.3	30
108	Topological Phases in Cove-Edged and Chevron Graphene Nanoribbons: Geometric Structures, [Formula: see text] Invariants, and Junction States. *Nano Letters*, **2018**, 18, 7247-7253	11.5	30

107	Bottom-up Assembly of Nanoporous Graphene with Emergent Electronic States. *Journal of the American Chemical Society*, **2020**, 142, 13507-13514	16.4	29
106	GW quasiparticle corrections to the LDA+U□GA+U electronic structure of bcc hydrogen. *Physical Review B*, **2008**, 77,	3.3	29
105	Excitons in carbon nanotubes: Diameter and chirality trends. *Physica Status Solidi (B): Basic Research* , **2007**, 244, 4016-4020	1.3	29
104	Temperature-Induced Topological Phase Transitions: Promoted versus Suppressed Nontrivial Topology. *Physical Review Letters*, **2016**, 117, 246401	7.4	29
103	Universal slow plasmons and giant field enhancement in atomically thin quasi-two-dimensional metals. *Nature Communications*, **2020**, 11, 1013	17.4	27
102	Spectroscopy of zigzag single-walled carbon nanotubes: Comparing femtosecond transient absorption spectra with ab initio calculations. *Physical Review B*, **2006**, 74,	3.3	27
101	Anisotropic Eliashberg theory and the two-band model for the superconducting properties of MgB2. *Physical Review B*, **2006**, 73,	3.3	27
100	Manipulation and characterization of aperiodical graphene structures created in a two-dimensional electron gas. *Physical Review Letters*, **2014**, 113, 196803	7.4	26
99	Length-Dependent Evolution of Type II Heterojunctions in Bottom-Up-Synthesized Graphene Nanoribbons. *Nano Letters*, **2019**, 19, 3221-3228	11.5	25
98	Automated construction of maximally localized Wannier functions: Optimized projection functions method. *Physical Review B*, **2015**, 92,	3.3	24
97	Ab initio calculations of pressure-induced structural phase transitions of GeTe. *Physical Review B*, **2010**, 82,	3.3	24
96	Electronic and optical properties of body-centered-tetragonal Si and Ge. *Physical Review B*, **2010**, 81,	3.3	24
95	Low-lying excited states in crystalline perylene. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 284-289	11.5	23
94	First-principles calculations of quasiparticle excitations of open-shell condensed matter systems. *Physical Review Letters*, **2012**, 109, 036406	7.4	23
93	Theoretical Models for the Optical Properties of Clusters and Nanostructures. *International Journal of Modern Physics B*, **1997**, 11, 2727-2776	1.1	23
92	Mechanism for bias-assisted indium mass transport on carbon nanotube surfaces. *Physical Review B*, **2005**, 72,	3.3	22
91	Ab initio quasiparticle band structure of ABA and ABC-stacked graphene trilayers. *Physical Review B* , **2014**, 89,	3.3	21
90	Effects of self-consistency and plasmon-pole models on GW calculations for closed-shell molecules. *Physical Review B*, **2014**, 90,	3.3	21

89	New Dirac fermions in periodically modulated bilayer graphene. *Nano Letters*, **2011**, 11, 2596-600	11.5	21
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