Steven G Louie

List of Publications by Year in Descending Order

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	Intervalley Excitonic Hybridization, Optical Selection Rules, and Imperfect Circular Dichroism in Monolayer h-BN.. *Physical Review Letters*, **2022**, 128, 047402	7.4	0
285	Multiple strong topological gaps and hexagonal warping in Bi4Te3. *Physical Review B*, **2022**, 105,	3.3	2
284	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	11.5	3
283	Spin splitting of dopant edge state in magnetic zigzag graphene nanoribbons.. *Nature*, **2021**, 600, 647-652	50.4	14
282	Topological Phases in Graphene Nanoribbons Tuned by Electric Fields. *Physical Review Letters*, **2021**, 127, 166401	7.4	3
281	Unmasking the Origin of Kinks in the Photoemission Spectra of Cuprate Superconductors. *Physical Review Letters*, **2021**, 126, 146401	7.4	4
280	Discovering and understanding materials through computation. *Nature Materials*, **2021**, 20, 728-735	27	13
279	Rational Passivation of Sulfur Vacancy Defects in Two-Dimensional Transition Metal Dichalcogenides. *ACS Nano*, **2021**, 15, 8780-8789	16.7	19
278	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,	11.5	4
277	Topology Classification using Chiral Symmetry and Spin Correlations in Graphene Nanoribbons. *Nano Letters*, **2021**, 21, 197-202	11.5	8
276	Solving the Bethe-Salpeter equation on a subspace: Approximations and consequences for low-dimensional materials. *Physical Review B*, **2021**, 103,	3.3	3
275	Imaging moir flat bands in three-dimensional reconstructed WSe/WS superlattices. *Nature Materials*, **2021**, 20, 945-950	27	41
274	Narrow-band high-lying excitons with negative-mass electrons in monolayer WSe. *Nature Communications*, **2021**, 12, 5500	17.4	5
273	Pseudo-atomic orbital behavior in graphene nanoribbons with four-membered rings.. *Science Advances*, **2021**, 7, eabl5892	14.3	1
272	Comparison of GW band structure to semiempirical approach for an FeSe monolayer. *Physical Review B*, **2020**, 101,	3.3	2
271	Reproducibility in G0W0 calculations for solids. *Computer Physics Communications*, **2020**, 255, 107242	4.2	14
270	Band gap renormalization, carrier mobilities, and the electron-phonon self-energy in crystalline naphthalene. *Physical Review B*, **2020**, 101,	3.3	5

269	Bottom-up Assembly of Nanoporous Graphene with Emergent Electronic States. *Journal of the American Chemical Society*, **2020**, 142, 13507-13514	16.4	29
268	Universal slow plasmons and giant field enhancement in atomically thin quasi-two-dimensional metals. *Nature Communications*, **2020**, 11, 1013	17.4	27
267	Covalent C-N Bond Formation through a Surface Catalyzed Thermal Cyclodehydrogenation. *Journal of the American Chemical Society*, **2020**, 142, 3696-3700	16.4	13
266	Polaron spectral properties in doped ZnO and SrTiO3 from first principles. *Physical Review Research* , **2020**, 2,	3.9	1
265	Direct observation of Klein tunneling in phononic crystals. *Science*, **2020**, 370, 1447-1450	33.3	30
264	A molecular shift register made using tunable charge patterns in one-dimensional molecular arrays on graphene. *Nature Electronics*, **2020**, 3, 598-603	28.4	3
263	Optical Imaging and Spectroscopy of Atomically Precise Armchair Graphene Nanoribbons. *Nano Letters*, **2020**, 20, 1124-1130	11.5	11
262	Strong correlations and orbital texture in single-layer 1T-TaSe2. *Nature Physics*, **2020**, 16, 218-224	16.2	56
261	Inducing metallicity in graphene nanoribbons via zero-mode superlattices. *Science*, **2020**, 369, 1597-1603	33.3	46
260	Predominance of non-adiabatic effects in zero-point renormalization of the electronic band gap. *Npj Computational Materials*, **2020**, 6,	10.9	20
259	Tunnel-FET Switching Is Governed by Non-Lorentzian Spectral Line Shape. *Proceedings of the IEEE*, **2020**, 108, 1235-1244	14.3	4
258	Nonuniversal critical behavior in disordered pseudospin-1 systems. *Physical Review B*, **2019**, 99,	3.3	6
257	Accelerating GW-Based Energy Level Alignment Calculations for Molecule-Metal Interfaces Using a Substrate Screening Approach. *Journal of Chemical Theory and Computation*, **2019**, 15, 4218-4227	6.4	16
256	Physical origin of giant excitonic and magneto-optical responses in two-dimensional ferromagnetic insulators. *Nature Communications*, **2019**, 10, 2371	17.4	42
255	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
254	Length-Dependent Evolution of Type II Heterojunctions in Bottom-Up-Synthesized Graphene Nanoribbons. *Nano Letters*, **2019**, 19, 3221-3228	11.5	25
253	Static subspace approximation for the evaluation of G0W0 quasiparticle energies within a sum-over-bands approach. *Physical Review B*, **2019**, 99,	3.3	2
252	Insulating titanium oxynitride for visible light photocatalysis. *Physical Review B*, **2019**, 99,	3.3	8

251	Geometry and electronic structure of iridium adsorbed on graphene. *Physical Review B*, **2019**, 99,	3.3	8
250	Layer-Dependent Electronic Structure of Atomically Resolved Two-Dimensional Gallium Selenide Telluride. *Nano Letters*, **2019**, 19, 1782-1787	11.5	9
249	A dielectric-defined lateral heterojunction in a monolayer semiconductor. *Nature Electronics*, **2019**, 2, 60-65	28.4	53
248	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
247	Valley-dependent exciton fine structure and Autler-Townes doublets from Berry phases in monolayer MoSe. *Nature Materials*, **2019**, 18, 1065-1070	27	18
246	Identifying substitutional oxygen as a prolific point defect in monolayer transition metal dichalcogenides. *Nature Communications*, **2019**, 10, 3382	17.4	117
245	Momentum-Resolved Dielectric Response of Free-Standing Mono-, Bi-, and Trilayer Black Phosphorus. *Nano Letters*, **2019**, 19, 8303-8310	11.5	12
244	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
243	Pseudospin-1 Physics of Photonic Crystals. *Research*, **2019**, 2019, 3054062	7.8	7
242	Large-scale GW calculations on pre-exascale HPC systems. *Computer Physics Communications*, **2019**, 235, 187-195	4.2	16
241	Exchange-driven intravalley mixing of excitons in monolayer transition metal dichalcogenides. *Nature Physics*, **2019**, 15, 228-232	16.2	43
240	Orbital Symmetry and the Optical Response of Single-Layer MX Monochalcogenides. *Nano Letters*, **2018**, 18, 1925-1929	11.5	30
239	Unifying Optical Selection Rules for Excitons in Two Dimensions: Band Topology and Winding Numbers. *Physical Review Letters*, **2018**, 120, 087402	7.4	34
238	Hierarchical On-Surface Synthesis of Graphene Nanoribbon Heterojunctions. *ACS Nano*, **2018**, 12, 2193-2200	13.7	55
237	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
236	Ultrasensitive tunability of the direct bandgap of 2D InSe flakes via strain engineering. *2D Materials* , **2018**, 5, 021002	5.9	53
235	Inversion symmetry and bulk Rashba effect in methylammonium lead iodide perovskite single crystals. *Nature Communications*, **2018**, 9, 1829	17.4	123
234	Topological band engineering of graphene nanoribbons. *Nature*, **2018**, 560, 204-208	50.4	287

233	Orbitally Matched Edge-Doping in Graphene Nanoribbons. *Journal of the American Chemical Society* , **2018**, 140, 807-813	16.4	45
232	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
231	Defect-Induced Modification of Low-Lying Excitons and Valley Selectivity in Monolayer Transition Metal Dichalcogenides. *Physical Review Letters*, **2018**, 121, 167402	7.4	69
230	A Structure Preserving Lanczos Algorithm for Computing the Optical Absorption Spectrum. *SIAM Journal on Matrix Analysis and Applications*, **2018**, 39, 683-711	1.5	10
229	Concentration Dependence of Dopant Electronic Structure in Bottom-up Graphene Nanoribbons. *Nano Letters*, **2018**, 18, 3550-3556	11.5	19
228	Nonuniform sampling schemes of the Brillouin zone for many-electron perturbation-theory calculations in reduced dimensionality. *Physical Review B*, **2017**, 95,	3.3	46
227	Spontaneous twisting of a collapsed carbon nanotube. *Nano Research*, **2017**, 10, 1942-1949	10	10
226	Ab initio Modelling of Plasmons in Metal-semiconductor Bilayer Transition-metal Dichalcogenide Heterostructures. *Israel Journal of Chemistry*, **2017**, 57, 540-546	3.4	4
225	Alternative structure of TiO2 with higher energy valence band edge. *Physical Review B*, **2017**, 95,	3.3	7
224	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
223	High thermoelectric power factor in two-dimensional crystals of MoS2. *Physical Review B*, **2017**, 95,	3.3	133
222	Discovery of intrinsic ferromagnetism in two-dimensional van der Waals crystals. *Nature*, **2017**, 546, 265-269	36.4	1890
221	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	11.5	20
220	Atomically precise graphene nanoribbon heterojunctions from a single molecular precursor. *Nature Nanotechnology*, **2017**, 12, 1077-1082	28.7	118
219	Dynamics of Symmetry-Breaking Stacking Boundaries in Bilayer MoS2. *Journal of Physical Chemistry C*, **2017**, 121, 22559-22566	3.8	17
218	Topological Phases in Graphene Nanoribbons: Junction States, Spin Centers, and Quantum Spin Chains. *Physical Review Letters*, **2017**, 119, 076401	7.4	151
217	Tunable excitons in bilayer graphene. *Science*, **2017**, 358, 907-910	33.3	89
216	Magnetic brightening and control of dark excitons in monolayer WSe. *Nature Nanotechnology*, **2017** , 12, 883-888	28.7	213

215	Symmetry rules shaping spin-orbital textures in surface states. *Physical Review B*, **2017**, 95,	3.3	8
214	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
213	Direct observation of the layer-dependent electronic structure in phosphorene. *Nature Nanotechnology*, **2017**, 12, 21-25	28.7	473
212	Origins of Singlet Fission in Solid Pentacene from an ab ̂initio Green's Function Approach. *Physical Review Letters*, **2017**, 119, 267401	7.4	42
211	Quasiparticle energies and dielectric functions of diamond polytypes. *Physical Review Materials*, **2017**, 1,	3.2	3
210	Real-space study of the optical absorption in alternative phases of silicon. *Physical Review Materials* , **2017**, 1,	3.2	2
209	Gate Switchable Transport and Optical Anisotropy in 90° Twisted Bilayer Black Phosphorus. *Nano Letters*, **2016**, 16, 5542-6	11.5	56
208	Tuning charge and correlation effects for a single molecule on a graphene device. *Nature Communications*, **2016**, 7, 13553	17.4	66
207	Dispersion and line shape of plasmon satellites in one, two, and three dimensions. *Physical Review B* , **2016**, 93,	3.3	12
206	Klein tunneling and supercollimation of pseudospin-1 electromagnetic waves. *Physical Review B*, **2016**, 93,	3.3	62
205	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
204	Screening and many-body effects in two-dimensional crystals: Monolayer MoS2. *Physical Review B*, **2016**, 93,	3.3	217
203	Proposal for a bulk material based on a monolayer FeSe on SrTiO3 high-temperature superconductor. *Physical Review B*, **2016**, 93,	3.3	12
202	Effective mass in bilayer graphene at low carrier densities: The role of potential disorder and electron-electron interaction. *Physical Review B*, **2016**, 94,	3.3	10
201	Bottom-Up Synthesis of N = 13 Sulfur-Doped Graphene Nanoribbons. *Journal of Physical Chemistry C*, **2016**, 120, 2684-2687	3.8	95
200	Fundamentals of Condensed Matter Physics **2016**,		96
199	Low rank approximation in G 0 W 0 calculations. *Science China Mathematics*, **2016**, 59, 1593-1612	0.8	10
198	Temperature-Induced Topological Phase Transitions: Promoted versus Suppressed Nontrivial Topology. *Physical Review Letters*, **2016**, 117, 246401	7.4	29

197	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
196	Automated construction of maximally localized Wannier functions for bands with nontrivial topology. *Physical Review B*, **2016**, 94,	3.3	3
195	Formation and Dynamics of Electron-Irradiation-Induced Defects in Hexagonal Boron Nitride at Elevated Temperatures. *Nano Letters*, **2016**, 16, 7142-7147	11.5	39
194	Electrostatically Driven Nanoballoon Actuator. *Nano Letters*, **2016**, 16, 6787-6791	11.5	13
193	Ab initio electronic relaxation times and transport in noble metals. *Physical Review B*, **2016**, 94,	3.3	40
192	Molecular bandgap engineering of bottom-up synthesized graphene nanoribbon heterojunctions. *Nature Nanotechnology*, **2015**, 10, 156-60	28.7	340
191	Tunable Magnetism and Half-Metallicity in Hole-Doped Monolayer GaSe. *Physical Review Letters*, **2015**, 114, 236602	7.4	257
190	Satellite band structure in silicon caused by electron-plasmon coupling. *Physical Review B*, **2015**, 91,	3.3	36
189	Site-Specific Substitutional Boron Doping of Semiconducting Armchair Graphene Nanoribbons. *Journal of the American Chemical Society*, **2015**, 137, 8872-5	16.4	177
188	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
187	Probing the role of interlayer coupling and coulomb interactions on electronic structure in few-layer MoSe$_2$ nanostructures. *Nano Letters*, **2015**, 15, 2594-9	11.5	110
186	Molecular Self-Assembly in a Poorly Screened Environment: F4TCNQ on Graphene/BN. *ACS Nano*, **2015**, 9, 12168-73	16.7	42
185	GW100: Benchmarking G0W0 for Molecular Systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 5665-87	6.4	207
184	Recent Advances in Two-Dimensional Materials beyond Graphene. *ACS Nano*, **2015**, 9, 11509-39	16.7	1581
183	Large electron–phonon interactions from FeSe phonons in a monolayer. *New Journal of Physics*, **2015**, 17, 073027	2.9	61
182	SU(4) symmetry breaking revealed by magneto-optical spectroscopy in epitaxial graphene. *Physical Review B*, **2015**, 91,	3.3	2
181	Automated construction of maximally localized Wannier functions: Optimized projection functions method. *Physical Review B*, **2015**, 92,	3.3	24
180	Theory and computation of hot carriers generated by surface plasmon polaritons in noble metals. *Nature Communications*, **2015**, 6, 7044	17.4	238

179	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
178	Numerical integration for ab initio many-electron self energy calculations within the GW approximation. *Journal of Computational Physics*, **2015**, 286, 1-13	4.1	11
177	First-principles theory of electron-spin fluctuation coupling and superconducting instabilities in iron selenide. *Physical Review B*, **2015**, 91,	3.3	12
176	Ab initio quasiparticle band structure of ABA and ABC-stacked graphene trilayers. *Physical Review B* , **2014**, 89,	3.3	21
175	Manipulation and characterization of aperiodical graphene structures created in a two-dimensional electron gas. *Physical Review Letters*, **2014**, 113, 196803	7.4	26
174	Three-dimensional spirals of atomic layered MoS2. *Nano Letters*, **2014**, 14, 6418-23	11.5	136
173	First-principles DFT+GW study of oxygen vacancies in rutile TiO2. *Physical Review B*, **2014**, 89,	3.3	75
172	Effects of self-consistency and plasmon-pole models on GW calculations for closed-shell molecules. *Physical Review B*, **2014**, 90,	3.3	21
171	Probing excitonic dark states in single-layer tungsten disulphide. *Nature*, **2014**, 513, 214-8	50.4	672
170	Giant bandgap renormalization and excitonic effects in a monolayer transition metal dichalcogenide semiconductor. *Nature Materials*, **2014**, 13, 1091-5	27	1150
169	ab initio study of hot carriers in the first picosecond after sunlight absorption in silicon. *Physical Review Letters*, **2014**, 112, 257402	7.4	166
168	Electron supercollimation in graphene and Dirac fermion materials using one-dimensional disorder potentials. *Physical Review Letters*, **2014**, 113, 026802	7.4	20
167	Imaging and tuning molecular levels at the surface of a gated graphene device. *ACS Nano*, **2014**, 8, 5395-401	10.7	31
166	Tuning Many-Body Interactions in Graphene: The Effects of Doping on Excitons and Carrier Lifetimes. *Physical Review Letters*, **2014**, 112,	7.4	57
165	Band offsets in c-Si/Si-XII heterojunctions. *Solid State Communications*, **2014**, 191, 6-9	1.6	
164	Excitonic Dark States in Single Atomic Layer of Transition Metal Dichalcogenide **2014**,		1
163	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
162	Improved quasiparticle wave functions and mean field for G0W0 calculations: Initialization with the COHSEX operator. *Physical Review B*, **2014**, 90,	3.3	14

161	Effect of spin fluctuations on quasiparticle excitations: First-principles theory and application to sodium and lithium. *Physical Review B*, **2014**, 89,	3.3	6
160	Optical spectrum of MoS2: many-body effects and diversity of exciton states. *Physical Review Letters*, **2013**, 111, 216805	7.4	1031
159	Photoelectron spin-flipping and texture manipulation in a topological insulator. *Nature Physics*, **2013**, 9, 293-298	16.2	152
158	Observing atomic collapse resonances in artificial nuclei on graphene. *Science*, **2013**, 340, 734-7	33.3	175
157	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
156	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
155	Intermolecular interactions and substrate effects for an adamantane monolayer on a Au(111) surface. *Physical Review B*, **2013**, 88,	3.3	4
154	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
153	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	4.2	530
152	Phonon-assisted optical absorption in silicon from first principles. *Physical Review Letters*, **2012**, 108, 167402	7.4	110
151	Anomalous insulator-metal transition in boron nitride-graphene hybrid atomic layers. *Physical Review B*, **2012**, 86,	3.3	41
150	Spin polarization of photoelectrons from topological insulators. *Physical Review Letters*, **2012**, 109, 097601	7.4	82
149	Mechanism for optical initialization of spin in NV□center in diamond. *Physical Review B*, **2012**, 86,	3.3	37
148	Inelastic carrier lifetime in bilayer graphene. *Applied Physics Letters*, **2012**, 100, 032106	3.4	4
147	First-principles calculations of quasiparticle excitations of open-shell condensed matter systems. *Physical Review Letters*, **2012**, 109, 036406	7.4	23
146	Quasiparticle effects in the bulk and surface-state bands of Bi2Se3 and Bi2Te3 topological insulators. *Physical Review B*, **2012**, 85,	3.3	101
145	Resonant excitation of graphene k-phonon and intra-landau-level excitons in magneto-optical spectroscopy [corrected]. *Physical Review Letters*, **2012**, 108, 247401	7.4	10
144	Enhanced electron-phonon coupling near the lattice instability of superconducting NbC1□Nx from density-functional calculations. *Physical Review B*, **2011**, 84,	3.3	15

143	New Dirac fermions in periodically modulated bilayer graphene. *Nano Letters*, **2011**, 11, 2596-600	11.5	21
142	Gate-controlled ionization and screening of cobalt adatoms on a graphene surface. *Nature Physics*, **2011**, 7, 43-47	16.2	198
141	Spatially resolving edge states of chiral graphene nanoribbons. *Nature Physics*, **2011**, 7, 616-620	16.2	557
140	Theory of magnetic edge states in chiral graphene nanoribbons. *Physical Review B*, **2011**, 84,	3.3	96
139	Excitonic effects in the optical properties of a SiC sheet and nanotubes. *Physical Review B*, **2011**, 84,	3.3	108
138	Quasiparticle excitations and charge transition levels of oxygen vacancies in hafnia. *Physical Review Letters*, **2011**, 107, 216803	7.4	50
137	Fermi surfaces and quantum oscillations in the underdoped high-Tc superconductors YBa2Cu3O6.5 and YBa2Cu4O8. *Physical Review B*, **2011**, 84,	3.3	6
136	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	3	16
135	Direct measurement of quantum phases in graphene via photoemission spectroscopy. *Physical Review B*, **2011**, 84,	3.3	64
134	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
133	Ab initio calculations of pressure-induced structural phase transitions of GeTe. *Physical Review B*, **2010**, 82,	3.3	24
132	Quasiparticle electronic structure of bismuth telluride in the GW approximation. *Physical Review B*, **2010**, 82,	3.3	50
131	Selective functionalization of halogens on zigzag graphene nanoribbons: A route to the separation of zigzag graphene nanoribbons. *Applied Physics Letters*, **2010**, 97, 233101	3.4	21
130	Tunable excitons in biased bilayer graphene. *Nano Letters*, **2010**, 10, 426-31	11.5	66
129	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
128	GW method with the self-consistent Sternheimer equation. *Physical Review B*, **2010**, 81,	3.3	98
127	Electronic and optical properties of body-centered-tetragonal Si and Ge. *Physical Review B*, **2010**, 81,	3.3	24
126	Electron-phonon coupling in C60 using hybrid functionals. *Physical Review B*, **2010**, 81,	3.3	39

125	Quasiparticle band gap of ZnO: high accuracy from the conventional G₀W₀ approach. *Physical Review Letters*, **2010**, 105, 146401	7.4	180
124	Electron-phonon renormalization of the direct band gap of diamond. *Physical Review Letters*, **2010**, 105, 265501	7.4	192
123	Calcium-decorated graphene-based nanostructures for hydrogen storage. *Nano Letters*, **2010**, 10, 793-8	11.5	300
122	Graphene Dirac fermions in one-dimensional inhomogeneous field profiles: Transforming magnetic to electric field. *Physical Review B*, **2010**, 81,	3.3	80
121	Observation of carrier-density-dependent many-body effects in graphene via tunneling spectroscopy. *Physical Review Letters*, **2010**, 104, 036805	7.4	96
120	Topological defects in graphene: Dislocations and grain boundaries. *Physical Review B*, **2010**, 81,	3.3	571
119	EPW: A program for calculating the electron–phonon coupling using maximally localized Wannier functions. *Computer Physics Communications*, **2010**, 181, 2140-2148	4.2	225
118	Prediction of superconducting properties of CaB2 using anisotropic Eliashberg theory. *Physical Review B*, **2009**, 80,	3.3	15
117	Angle-resolved photoemission spectra of graphene from first-principles calculations. *Nano Letters*, **2009**, 9, 4234-9	11.5	93
116	Mechanically controlled binary conductance switching of a single-molecule junction. *Nature Nanotechnology*, **2009**, 4, 230-4	28.7	515
115	Electron-hole interaction in carbon nanotubes: novel screening and exciton excitation spectra. *Nano Letters*, **2009**, 9, 1330-4	11.5	57
114	Calcium-decorated carbon nanotubes for high-capacity hydrogen storage: First-principles calculations. *Physical Review B*, **2009**, 80,	3.3	135
113	First-principles study of electron linewidths in graphene. *Physical Review Letters*, **2009**, 102, 076803	7.4	65
112	Excitonic effects on the optical response of graphene and bilayer graphene. *Physical Review Letters*, **2009**, 103, 186802	7.4	509
111	Landau levels and quantum Hall effect in graphene superlattices. *Physical Review Letters*, **2009**, 103, 046808	7.4	125
110	Making massless Dirac fermions from a patterned two-dimensional electron gas. *Nano Letters*, **2009**, 9, 1793-7	11.5	120
109	Anisotropic Eliashberg theory for superconductivity in compressed and doped MgB2. *Physical Review B*, **2009**, 79,	3.3	13
108	GW approach to Anderson model out of equilibrium: Coulomb blockade and false hysteresis in the IV characteristics. *Physical Review B*, **2009**, 79,	3.3	47

107	Small phonon contribution to the photoemission kink in the copper oxide superconductors. *Nature*, **2008**, 452, 975-8	50.4	135
106	Anisotropic behaviours of massless Dirac fermions in graphene under periodic potentials. *Nature Physics*, **2008**, 4, 213-217	16.2	531
105	Electron beam supercollimation in graphene superlattices. *Nano Letters*, **2008**, 8, 2920-4	11.5	223
104	Optimization of metal dispersion in doped graphitic materials for hydrogen storage. *Physical Review B*, **2008**, 78,	3.3	105
103	GW quasiparticle corrections to the LDA+U□GA+U electronic structure of bcc hydrogen. *Physical Review B*, **2008**, 77,	3.3	29
102	Electron-phonon interactions in graphene, bilayer graphene, and graphite. *Nano Letters*, **2008**, 8, 4229-33	11.5	138
101	New generation of massless Dirac fermions in graphene under external periodic potentials. *Physical Review Letters*, **2008**, 101, 126804	7.4	316
100	Negative differential resistance in carbon atomic wire-carbon nanotube junctions. *Nano Letters*, **2008**, 8, 2900-5	11.5	152
99	Van Hove singularity and apparent anisotropy in the electron-phonon interaction in graphene. *Physical Review B*, **2008**, 77,	3.3	46
98	Contact dependence of the conductance of H2 molecular junctions from first principles. *Physical Review B*, **2008**, 77,	3.3	10
97	Low-energy structures of K atoms in expanded K3C60 monolayers: Ab initio pseudopotential density-functional calculations. *Physical Review B*, **2008**, 77,	3.3	3
96	Amine-gold linked single-molecule circuits: experiment and theory. *Nano Letters*, **2007**, 7, 3477-82	11.5	403
95	Bound excitons in metallic single-walled carbon nanotubes. *Nano Letters*, **2007**, 7, 1626-30	11.5	93
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