

# Feliciano Giustino

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

164 papers	15,554 citations	54 h-index	124 g-index
179 ext. papers	19,264 ext. citations	7.5 avg, IF	7.33 L-index

#	Paper	IF	Citations
164	CeTaN3 and CeNbN3: Prospective Nitride Perovskites with Optimal Photovoltaic Band Gaps. <i>Chemistry of Materials</i> , <b>2022</b> , 34, 2107-2122	9.6	2
163	Dynamic Rashba-Dresselhaus Effect.. <i>Physical Review Letters</i> , <b>2021</b> , 127, 237601	7.4	1
162	Monolayer 1T-NbSe as a 2D-correlated magnetic insulator. <i>Science Advances</i> , <b>2021</b> , 7, eabi6339	14.3	6
161	Multiphonon diffuse scattering in solids from first principles: Application to layered crystals and two-dimensional materials. <i>Physical Review B</i> , <b>2021</b> , 104,	3.3	5
160	Efficient First-Principles Methodology for the Calculation of the All-Phonon Inelastic Scattering in Solids. <i>Physical Review Letters</i> , <b>2021</b> , 127, 207401	7.4	5
159	First-principles predictions of Hall and drift mobilities in semiconductors. <i>Physical Review Research</i> , <b>2021</b> , 3,	3.9	5
158	GW band structure of monolayer MoS2 using the SternheimerGW method and effect of dielectric environment. <i>Physical Review B</i> , <b>2021</b> , 103,	3.3	1
157	Exciton-Phonon Interactions in Monolayer Germanium Selenide from First Principles. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 3802-3808	6.4	4
156	Limits to Electrical Mobility in Lead-Halide Perovskite Semiconductors. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 3607-3617	6.4	14
155	Phonon-Limited Mobility and Electron-Phonon Coupling in Lead-Free Halide Double Perovskites. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 4474-4482	6.4	12
154	Crystallographic, Optical, and Electronic Properties of the Cs2AgBi1-xInxBBr6 Double Perovskite: Understanding the Fundamental Photovoltaic Efficiency Challenges. <i>ACS Energy Letters</i> , <b>2021</b> , 6, 1073-1081	20.1	10
153	Electronic Structure and Electron-Transport Properties of Three Metal Hexacyanoferrates. <i>Chemistry of Materials</i> , <b>2021</b> , 33, 7067-7074	9.6	3
152	First-principles study of electron transport in ScN. <i>Physical Review B</i> , <b>2021</b> , 104,	3.3	1
151	Ultrafast photo-induced phonon hardening due to Pauli blocking in MAPbI3 single-crystal and polycrystalline perovskites. <i>JPhys Materials</i> , <b>2021</b> , 4, 044017	4.2	0
150	Ruddlesden-Popper-Phase Hybrid Halide Perovskite/Small-Molecule Organic Blend Memory Transistors. <i>Advanced Materials</i> , <b>2021</b> , 33, e2003137	24	17
149	Spin waves in metallic iron and nickel measured by soft x-ray resonant inelastic scattering. <i>Physical Review B</i> , <b>2020</b> , 102,	3.3	3
148	Superconducting properties of MoTe2 from ab initio anisotropic Migdal-Eliashberg theory. <i>Physical Review B</i> , <b>2020</b> , 101,	3.3	3

147	Many-body renormalization of the electron effective mass of InSe. <i>Physical Review B</i> , <b>2020</b> , 101,	3.3	3
146	Electron-polaron dichotomy of charge carriers in perovskite oxides. <i>Communications Physics</i> , <b>2020</b> , 3,	5.4	7
145	Theory of the special displacement method for electronic structure calculations at finite temperature. <i>Physical Review Research</i> , <b>2020</b> , 2,	3.9	23
144	Structural, electronic, elastic, power, and transport properties of $\text{BaTiO}_3$ from first principles. <i>Physical Review Research</i> , <b>2020</b> , 2,	3.9	20
143	Many-Body Calculations of Plasmon and Phonon Satellites in Angle-Resolved Photoelectron Spectra Using the Cumulant Expansion Approach <b>2020</b> , 341-365		
142	Hybrid Halide Perovskites: Fundamental Theory and Materials Design <b>2020</b> , 295-324		2
141	First-principles calculations of charge carrier mobility and conductivity in bulk semiconductors and two-dimensional materials. <i>Reports on Progress in Physics</i> , <b>2020</b> , 83, 036501	14.4	71
140	Theory and Computation of Hall Scattering Factor in Graphene. <i>Nano Letters</i> , <b>2020</b> , 20, 8861-8865	11.5	2
139	Intrinsic quantum confinement in formamidinium lead triiodide perovskite. <i>Nature Materials</i> , <b>2020</b> , 19, 1201-1206	27	10
138	SternheimerGW: A program for calculating GW quasiparticle band structures and spectral functions without unoccupied states. <i>Computer Physics Communications</i> , <b>2020</b> , 247, 106856	4.2	7
137	The 2021 quantum materials roadmap. <i>JPhys Materials</i> , <b>2020</b> , 3, 042006	4.2	48
136	Hole mobility of strained GaN from first principles. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	38
135	Route to High Hole Mobility in GaN via Reversal of Crystal-Field Splitting. <i>Physical Review Letters</i> , <b>2019</b> , 123, 096602	7.4	31
134	Ab initio theory of polarons: Formalism and applications. <i>Physical Review B</i> , <b>2019</b> , 99,	3.3	32
133	Polarons from First Principles, without Supercells. <i>Physical Review Letters</i> , <b>2019</b> , 122, 246403	7.4	32
132	Manipulating surface magnetic order in iron telluride. <i>Science Advances</i> , <b>2019</b> , 5, eaav3478	14.3	9
131	Oxide Analogs of Halide Perovskites and the New Semiconductor BaAgIO. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 1722-1728	6.4	18
130	Dimensional Crossover in the Carrier Mobility of Two-Dimensional Semiconductors: The Case of InSe. <i>Nano Letters</i> , <b>2019</b> , 19, 1774-1781	11.5	34

129	Coexistence of Superconductivity with Enhanced Charge Density Wave Order in the Two-Dimensional Limit of TaSe. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 4076-4081	6.4	20
128	Trellises of Molecular Oxygen on Anatase TiO <sub>2</sub> (101). <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 26170-26177	17.7	1
127	Slot-Die-Printed Two-Dimensional ZrS Charge Transport Layer for Perovskite Light-Emitting Diodes. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 48021-48028	9.5	10
126	Origin of Low Carrier Mobilities in Halide Perovskites. <i>ACS Energy Letters</i> , <b>2019</b> , 4, 456-463	20.1	79
125	Universal Scaling of Intrinsic Resistivity in Two-Dimensional Metallic Borophene. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 4585-4589	16.4	18
124	Universal Scaling of Intrinsic Resistivity in Two-Dimensional Metallic Borophene. <i>Angewandte Chemie</i> , <b>2018</b> , 130, 4675-4679	3.6	4
123	Electron-plasmon and electron-phonon satellites in the angle-resolved photoelectron spectra of n-doped anatase TiO <sub>2</sub> . <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	14
122	High-Efficiency Fullerene Solar Cells Enabled by a Spontaneously Formed Mesoporous CuSCN-Nanowire Heterointerface. <i>Advanced Science</i> , <b>2018</b> , 5, 1700980	13.6	15
121	Bimolecular recombination in methylammonium lead triiodide perovskite is an inverse absorption process. <i>Nature Communications</i> , <b>2018</b> , 9, 293	17.4	175
120	Ab initio calculation of spin fluctuation spectra using time-dependent density functional perturbation theory, plane waves, and pseudopotentials. <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	13
119	Oxygen redox chemistry without excess alkali-metal ions in Na[MgMn]O. <i>Nature Chemistry</i> , <b>2018</b> , 10, 288-295	17.6	281
118	Towards predictive many-body calculations of phonon-limited carrier mobilities in semiconductors. <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	128
117	Graphene Oxide/Perovskite Interfaces For Photovoltaics. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 16715-16726	15.7	16726
116	Cubic or Orthorhombic? Revealing the Crystal Structure of Metastable Black-Phase CsPbI <sub>3</sub> by Theory and Experiment. <i>ACS Energy Letters</i> , <b>2018</b> , 3, 1787-1794	20.1	292
115	The geometric blueprint of perovskites. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2018</b> , 115, 5397-5402	11.5	70
114	Quasiparticle GW band structures and Fermi surfaces of bulk and monolayer NbS <sub>2</sub> . <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	10
113	Carrier Lifetimes and Polaronic Mass Enhancement in the Hybrid Halide Perovskite CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> from Multiphonon Fröhlich Coupling. <i>Physical Review Letters</i> , <b>2018</b> , 121, 086402	7.4	48
112	Hybrid Halide Perovskites: Fundamental Theory and Materials Design <b>2018</b> , 1-30		4

111	Surface properties of lead-free halide double perovskites: Possible visible-light photo-catalysts for water splitting. <i>Applied Physics Letters</i> , <b>2018</b> , 112, 243901	3.4	34
110	Crossover from lattice to plasmonic polarons of a spin-polarised electron gas in ferromagnetic EuO. <i>Nature Communications</i> , <b>2018</b> , 9, 2305	17.4	19
109	Phase Diagrams and Stability of Lead-Free Halide Double Perovskites Cs <sub>2</sub> BB'X <sub>6</sub> : B = Sb and Bi, B' = Cu, Ag, and Au, and X = Cl, Br, and I. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 158-170	3.8	91
108	Halide Perovskites: Interfaces Between Graphene-Related Materials and MAPbI <sub>3</sub> : Insights from First-Principles (Adv. Mater. Interfaces 22/2018). <i>Advanced Materials Interfaces</i> , <b>2018</b> , 5, 1870110	4.6	1
107	Many-Body Calculations of Plasmon and Phonon Satellites in Angle-Resolved Photoelectron Spectra Using the Cumulant Expansion Approach <b>2018</b> , 1-25		
106	Raman Spectrum of the Organic-Inorganic Halide Perovskite CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> from First Principles and High-Resolution Low-Temperature Raman Measurements. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 21703-21717	3.8	53
105	Atomic Structure of Water Monolayer on Anatase TiO <sub>2</sub> (101) Surface. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 11954-11960	3.8	12
104	CsInAgCl: A New Lead-Free Halide Double Perovskite with Direct Band Gap. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 772-778	6.4	494
103	Electron-phonon interactions from first principles. <i>Reviews of Modern Physics</i> , <b>2017</b> , 89,	40.5	538
102	Solution-Processed Cesium Hexabromopalladate(IV), CsPdBr <sub>6</sub> , for Optoelectronic Applications. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 6030-6033	16.4	134
101	Single-Molecule Vibrational Spectroscopy of H <sub>2</sub> O on Anatase TiO <sub>2</sub> (101). <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 1182-1187	3.8	21
100	Advanced capabilities for materials modelling with Quantum ESPRESSO. <i>Journal of Physics Condensed Matter</i> , <b>2017</b> , 29, 465901	1.8	2275
99	Origin of Superconductivity and Latent Charge Density Wave in NbS <sub>2</sub> . <i>Physical Review Letters</i> , <b>2017</b> , 119, 087003	7.4	66
98	Route to Stable Lead-Free Double Perovskites with the Electronic Structure of CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> : A Case for Mixed-Cation [Cs/CH <sub>3</sub> NH/CH(NH <sub>2</sub> )]InBiBr. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 3917-3924	6.4	71
97	Van der Waals Interactions and Anharmonicity in the Lattice Vibrations, Dielectric Constants, Effective Charges, and Infrared Spectra of the Organic-Inorganic Halide Perovskite CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> . <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 18459-18471	3.8	22
96	Origin of the crossover from polarons to Fermi liquids in transition metal oxides. <i>Nature Communications</i> , <b>2017</b> , 8, 15769	17.4	79
95	Nonadiabatic Kohn Anomaly in Heavily Boron-Doped Diamond. <i>Physical Review Letters</i> , <b>2017</b> , 119, 017001	7.4	25
94	One-shot calculation of temperature-dependent optical spectra and phonon-induced band-gap renormalization. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	77

93	EPW: Electron-phonon coupling, transport and superconducting properties using maximally localized Wannier functions. <i>Computer Physics Communications</i> , <b>2016</b> , 209, 116-133	4.2	433
92	Electron-phonon coupling in hybrid lead halide perovskites. <i>Nature Communications</i> , <b>2016</b> , 7,	17.4	668
91	Toward Lead-Free Perovskite Solar Cells. <i>ACS Energy Letters</i> , <b>2016</b> , 1, 1233-1240	20.1	636
90	Perovskite-perovskite tandem photovoltaics with optimized band gaps. <i>Science</i> , <b>2016</b> , 354, 861-865	33.3	865
89	Band Gaps of the Lead-Free Halide Double Perovskites Cs <sub>2</sub> BiAgCl <sub>6</sub> and Cs <sub>2</sub> BiAgBr <sub>6</sub> from Theory and Experiment. <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 2579-85	6.4	395
88	Confinement Effects in Low-Dimensional Lead Iodide Perovskite Hybrids. <i>Chemistry of Materials</i> , <b>2016</b> , 28, 4554-4562	9.6	203
87	Energy-level alignment and open-circuit voltage at graphene/polymer interfaces: theory and experiment. <i>2D Materials</i> , <b>2016</b> , 3, 015003	5.9	7
86	Computational Screening of Homovalent Lead Substitution in Organic-Inorganic Halide Perovskites. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 166-173	3.8	162
85	Lead-Free Halide Double Perovskites via Heterovalent Substitution of Noble Metals. <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 1254-9	6.4	567
84	Electron-phonon interaction and pairing mechanism in superconducting Ca-intercalated bilayer graphene. <i>Scientific Reports</i> , <b>2016</b> , 6, 21414	4.9	49
83	The GW plus cumulant method and plasmonic polarons: application to the homogeneous electron gas*. <i>European Physical Journal B</i> , <b>2016</b> , 89, 1	1.2	14
82	Modelling graphene quantum dot functionalization via ethylene-dinitrobenzoyl. <i>Applied Physics Letters</i> , <b>2016</b> , 108, 123902	3.4	1
81	Theory of electron-plasmon coupling in semiconductors. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	29
80	On the combined use of GW approximation and cumulant expansion in the calculations of quasiparticle spectra: The paradigm of Si valence bands. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	28
79	Ferroelectric Graphene-Perovskite Interfaces. <i>Journal of Physical Chemistry Letters</i> , <b>2015</b> , 6, 2496-502	6.4	60
78	Band structures of plasmonic polarons. <i>Physical Review Letters</i> , <b>2015</b> , 114, 146404	7.4	50
77	Vibrational Properties of the Organic-Inorganic Halide Perovskite CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> from Theory and Experiment: Factor Group Analysis, First-Principles Calculations, and Low-Temperature Infrared Spectra. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 25703-25718	3.8	220
76	Graphene-based technologies for energy applications, challenges and perspectives. <i>2D Materials</i> , <b>2015</b> , 2, 030204	5.9	62

75	GW Band Structures and Carrier Effective Masses of CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> and Hypothetical Perovskites of the Type APbI <sub>3</sub> : A = NH <sub>4</sub> , PH <sub>4</sub> , AsH <sub>4</sub> , and SbH <sub>4</sub> . <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 25209-25219	3.8	113
74	Excitons in one-dimensional van der Waals materials: Sb <sub>2</sub> S <sub>3</sub> nanoribbons. <i>Physical Review B</i> , <b>2015</b> , 92,	3.3	21
73	Fröhlich Electron-Phonon Vertex from First Principles. <i>Physical Review Letters</i> , <b>2015</b> , 115, 176401	7.4	165
72	Stochastic Approach to Phonon-Assisted Optical Absorption. <i>Physical Review Letters</i> , <b>2015</b> , 115, 177401	7.4	63
71	Spectral fingerprints of electron-plasmon coupling. <i>Physical Review B</i> , <b>2015</b> , 92,	3.3	19
70	Theory of Electromagnons in CuO. <i>Physical Review Letters</i> , <b>2015</b> , 114, 197201	7.4	13
69	First-principles study of structurally modulated multiferroic CaMn <sub>7</sub> O <sub>12</sub> . <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	12
68	Two-gap superconductivity in heavily n-doped graphene: Ab initio Migdal-Eliashberg theory. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	51
67	Unified theory of electron-phonon renormalization and phonon-assisted optical absorption. <i>Journal of Physics Condensed Matter</i> , <b>2014</b> , 26, 365503	1.8	42
66	CaBaCo <sub>4</sub> O <sub>7</sub> : A ferrimagnetic pyroelectric. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	32
65	Atomic-scale observation of multiconformational binding and energy level alignment of ruthenium-based photosensitizers on TiO <sub>2</sub> anatase. <i>Nano Letters</i> , <b>2014</b> , 14, 563-9	11.5	60
64	First-principles study of multiferroic RbFe(MoO <sub>4</sub> ) <sub>2</sub> . <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	5
63	Structure of a Water Monolayer on the Anatase TiO <sub>2</sub> (101) Surface. <i>Physical Review Applied</i> , <b>2014</b> , 2,	4.3	34
62	TiO <sub>2</sub> anatase with a bandgap in the visible region. <i>Nano Letters</i> , <b>2014</b> , 14, 6533-8	11.5	384
61	Time-dependent density functional theory using atomic orbitals and the self-consistent Sternheimer equation. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	14
60	GW quasiparticle band gap of the hybrid organic-inorganic perovskite CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> : Effect of spin-orbit interaction, semicore electrons, and self-consistency. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	101
59	Steric engineering of metal-halide perovskites with tunable optical band gaps. <i>Nature Communications</i> , <b>2014</b> , 5, 5757	17.4	605
58	Linear optical response of finite systems using multishift linear system solvers. <i>Journal of Chemical Physics</i> , <b>2014</b> , 141, 044117	3.9	13



57	GW quasiparticle band structures of stibnite, antimonelite, bismuthinite, and guanajuatite. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	142
56	Anisotropic Migdal-Eliashberg theory using Wannier functions. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	124
55	Ab initio Sternheimer-GW method for quasiparticle calculations using plane waves. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	35
54	Quantum nuclear dynamics in the photophysics of diamondoids. <i>Nature Communications</i> , <b>2013</b> , 4, 2006	17.4	76
53	Strong carrier lifetime enhancement in GaAs nanowires coated with semiconducting polymer. <i>Nano Letters</i> , <b>2012</b> , 12, 6293-301	11.5	52
52	Ultrafast entangling gates between nuclear spins using photoexcited triplet states. <i>Nature Physics</i> , <b>2012</b> , 8, 596-600	16.2	39
51	Performance of local orbital basis sets in the self-consistent Sternheimer method for dielectric matrices of extended systems. <i>European Physical Journal B</i> , <b>2012</b> , 85, 1	1.2	6
50	Quantitative analysis of valence photoemission spectra and quasiparticle excitations at chromophore-semiconductor interfaces. <i>Physical Review Letters</i> , <b>2012</b> , 109, 116801	7.4	24
49	Dielectric screening in extended systems using the self-consistent Sternheimer equation and localized basis sets. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	12
48	Inelastic carrier lifetime in bilayer graphene. <i>Applied Physics Letters</i> , <b>2012</b> , 100, 032106	3.4	4
47	GW quasiparticle bandgaps of anatase TiO <sub>2</sub> starting from DFT + U. <i>Journal of Physics Condensed Matter</i> , <b>2012</b> , 24, 202201	1.8	52
46	Ideal Energy-Level Alignment at the ZnO/P3HT Photovoltaic Interface. <i>Advanced Functional Materials</i> , <b>2012</b> , 22, 5089-5095	15.6	53
45	Dislocation-driven deformations in graphene. <i>Science</i> , <b>2012</b> , 337, 209-12	33.3	295
44	First-principles investigation of hyperfine interactions for nuclear spin entanglement in photoexcited fullerenes. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	9
43	Modeling the role of the fluorine dopant in the magnetic phase diagram of LaFeAsO <sub>1-x</sub> F <sub>x</sub> superconductors. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	1
42	Structural and Electronic Properties of Semiconductor-Sensitized Solar-Cell Interfaces. <i>Advanced Functional Materials</i> , <b>2011</b> , 21, 4663-4667	15.6	110
41	Solar Cells: Structural and Electronic Properties of Semiconductor-Sensitized Solar-Cell Interfaces (Adv. Funct. Mater. 24/2011). <i>Advanced Functional Materials</i> , <b>2011</b> , 21, 4798-4798	15.6	1
40	O 1s core-level shifts at the anatase TiO <sub>2</sub> (101)/N <sub>3</sub> photovoltaic interface: Signature of H-bonded supramolecular assembly. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	22



39	Publisher's Note: First-Principles Prediction of Doped Graphane as a High-Temperature Electron-Phonon Superconductor [Phys. Rev. Lett. 105, 037002 (2010)]. <i>Physical Review Letters</i> , <b>2010</b> , 105,	7.4	5
38	Entangling remote nuclear spins linked by a chromophore. <i>Physical Review Letters</i> , <b>2010</b> , 104, 200501	7.4	15
37	GW method with the self-consistent Sternheimer equation. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	98
36	First-principles prediction of doped graphane as a high-temperature electron-phonon superconductor. <i>Physical Review Letters</i> , <b>2010</b> , 105, 037002	7.4	140
35	Electron-phonon renormalization of the direct band gap of diamond. <i>Physical Review Letters</i> , <b>2010</b> , 105, 265501	7.4	192
34	EPW: A program for calculating the electron-phonon coupling using maximally localized Wannier functions. <i>Computer Physics Communications</i> , <b>2010</b> , 181, 2140-2148	4.2	225
33	Role of fluorine in the iron pnictides: phonon softening and effective hole doping. <i>Physical Review Letters</i> , <b>2009</b> , 102, 147003	7.4	15
32	Angle-resolved photoemission spectra of graphene from first-principles calculations. <i>Nano Letters</i> , <b>2009</b> , 9, 4234-9	11.5	93
31	First-principles study of electron linewidths in graphene. <i>Physical Review Letters</i> , <b>2009</b> , 102, 076803	7.4	65
30	Origin of superconductivity in boron-doped silicon carbide from first principles. <i>Physical Review B</i> , <b>2009</b> , 79,	3.3	26
29	Small phonon contribution to the photoemission kink in the copper oxide superconductors. <i>Nature</i> , <b>2008</b> , 452, 975-8	50.4	135
28	Electron-phonon interactions in graphene, bilayer graphene, and graphite. <i>Nano Letters</i> , <b>2008</b> , 8, 4229-33	11.5	138
27	First-principles theory of infrared absorption spectra at surfaces and interfaces: Application to the Si(100):H <sub>2</sub> O surface. <i>Physical Review B</i> , <b>2008</b> , 78,	3.3	6
26	First-principles study of superconductivity and Fermi-surface nesting in ultrahard transition metal carbides. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	24
25	Van Hove singularity and apparent anisotropy in the electron-phonon interaction in graphene. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	46
24	Band offsets at the Si/SiO <sub>2</sub> interface from many-body perturbation theory. <i>Physical Review Letters</i> , <b>2008</b> , 100, 186401	7.4	141
23	Electron-phonon interaction using Wannier functions. <i>Physical Review B</i> , <b>2007</b> , 76,	3.3	425
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20	Proton-induced fixed positive charge at the Si(100)-SiO <sub>2</sub> interface. <i>Physical Review Letters</i> , <b>2007</b> , 99, 126102	7.4	20
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17	DIELECTRIC AND INFRARED PROPERTIES OF ULTRATHIN SiO <sub>2</sub> LAYERS ON Si(100). <i>NATO Science Series Series II, Mathematics, Physics and Chemistry</i> , <b>2006</b> , 385-396		1
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14	Atomistic models of the Si(100)/SiO <sub>2</sub> interface: structural, electronic and dielectric properties. <i>Journal of Physics Condensed Matter</i> , <b>2005</b> , 17, S2065-S2074	1.8	41
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8	Dielectric effect of a thin SiO <sub>2</sub> interlayer at the interface between silicon and high-k oxides. <i>Microelectronic Engineering</i> , <b>2004</b> , 72, 299-303	2.5	24
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2	Dose and dose rate effects on NPN bipolar junction transistors irradiated at high temperature		1
1	Quasiparticle Band Structure and Phonon-Induced Band Gap Renormalization of the Lead-Free Halide Double Perovskite Cs <sub>2</sub> InAgCl <sub>6</sub> . <i>Journal of Physical Chemistry C</i> ,	3.8	5