Feliciano Giustino

List of Publications by Year
in descending order

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174 papers	23,095 citations	17405 63 h-index	7718 150 g-index
179 all docs	179 docs citations	179 times ranked	22820 citing authors

#	Article	IF	Citations
1	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	0.7	4,303
2	Perovskite-perovskite tandem photovoltaics with optimized band gaps. Science, 2016, 354, 861-865.	6.0	1,107
3	Electron-phonon interactions from first principles. Reviews of Modern Physics, 2017, 89, .	16.4	947
4	Electronâ€“phonon coupling in hybrid lead halide perovskites. Nature Communications, 2016, 7, .	5.8	919
5	Toward Lead-Free Perovskite Solar Cells. ACS Energy Letters, 2016, 1, 1233-1240.	8.8	848
6	Steric engineering of metal-halide perovskites with tunable optical band gaps. Nature Communications, 2014, 5, 5757.	5.8	787
7	EPW: Electronâ€“phonon coupling, transport and superconducting properties using maximally localized Wannier functions. Computer Physics Communications, 2016, 209, 116-133.	3.0	777
8	Lead-Free Halide Double Perovskites via Heterovalent Substitution of Noble Metals. Journal of Physical Chemistry Letters, 2016, 7, 1254-1259.	2.1	761
9	Cs₂InAgCl₆: A New Lead-Free Halide Double Perovskite with Direct Band Gap. Journal of Physical Chemistry Letters, 2017, 8, 772-778.	2.1	752
10	Electron-phonon interaction using Wannier functions. Physical Review B, 2007, 76, .	1.1	625
11	TiO₂ Anatase with a Bandgap in the Visible Region. Nano Letters, 2014, 14, 6533-6538.	4.5	531
12	Band Gaps of the Lead-Free Halide Double Perovskites Cs₂BiAgCl₆ and Cs₂BiAgBr₆ from Theory and Experiment. Journal of Physical Chemistry Letters, 2016, 7, 2579-2585.	2.1	529
13	Cubic or Orthorhombic? Revealing the Crystal Structure of Metastable Black-Phase CsPbI₃ by Theory and Experiment. ACS Energy Letters, 2018, 3, 1787-1794.	8.8	455
14	Oxygen redox chemistry without excess alkali-metal ions in Na2/3[Mg0.28Mn0.72]O2. Nature Chemistry, 2018, 10, 288-295.	6.6	414
15	Dislocation-Driven Deformations in Graphene. Science, 2012, 337, 209-212.	6.0	332
16	EPW: A program for calculating the electronâ€“phonon coupling using maximally localized Wannier functions. Computer Physics Communications, 2010, 181, 2140-2148.	3.0	324
17	Vibrational Properties of the Organicâ€“Inorganic Halide Perovskite CH₃NH₃PbI₃ from Theory and Experiment: Factor Group Analysis, First-Principles Calculations, and Low-Temperature Infrared Spectra. Journal of Physical Chemistry C, 2015, 119, 25703-25718.	1.5	276
18	Confinement Effects in Low-Dimensional Lead Iodide Perovskite Hybrids. Chemistry of Materials, 2016, 28, 4554-4562.	3.2	263

#	Article	IF	Citations
19	Bimolecular recombination in methylammonium lead triiodide perovskite is an inverse absorption process. Nature Communications, 2018, 9, 293.	5.8	243
20	Electron-Phonon Renormalization of the Direct Band Gap of Diamond. Physical Review Letters, 2010, 105, 265501.	2.9	241
21	FrÃ¶hlich Electron-Phonon Vertex from First Principles. Physical Review Letters, 2015, 115, 176401.	2.9	232
22	Towards predictive many-body calculations of phonon-limited carrier mobilities in semiconductors. Physical Review B, 2018, 97, .	1.1	224
23	Anisotropic Migdal-Eliashberg theory using Wannier functions. Physical Review B, 2013, 87, .	1.1	220
24	Computational Screening of Homovalent Lead Substitution in Organicâ€“Inorganic Halide Perovskites. Journal of Physical Chemistry C, 2016, 120, 166-173.	1.5	208
25	Solution-Processed Cesium Hexabromopalladate(IV), Cs₂PdBr₆, for Optoelectronic Applications. Journal of the American Chemical Society, 2017, 139, 6030-6033.	6.6	189
26	Velocity Renormalization and Carrier Lifetime in Graphene from the Electron-Phonon Interaction. Physical Review Letters, 2007, 99, 086804.	2.9	183
27	First-Principles Prediction of Doped Graphane as a High-Temperature Electron-Phonon Superconductor. Physical Review Letters, 2010, 105, 037002.	2.9	178
28	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>quasiparticle band structures of stibnite, antimonselite, bismuthinite, and guanajuatite. Physical Review B, 2013, 87, .	1.1	178
29	First-principles calculations of charge carrier mobility and conductivity in bulk semiconductors and two-dimensional materials. Reports on Progress in Physics, 2020, 83, 036501.	8.1	176
30	Small phonon contribution to the photoemission kink in the copper oxide superconductors. Nature, 2008, 452, 975-978.	13.7	157
31	Electronâ^'Phonon Interactions in Graphene, Bilayer Graphene, and Graphite. Nano Letters, 2008, 8, 4229-4233.	4.5	156
32	Band Offsets at the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Si</mml:mi><mml:mo>/</mml:mo><mml:msub><mml:mi>SiO</mml:mi><mml:mn>2</mml:mn></mml:msub> from Many-Body Perturbation Theory. Physical Review Letters, 2008, 100, 186401.	2.9	154
33	GW Band Structures and Carrier Effective Masses of CH₃NH₃PbI₃ and Hypothetical Perovskites of the Type APbI₃: A = NH₄, PH₄, AsH₄, and SbH₄. Journal of Physical Chemistry C, 2015, 119, 25209-25219.	1.5	144
34	The geometric blueprint of perovskites. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 5397-5402.	3.3	138
35	Electron-Phonon Interaction via Electronic and Lattice Wannier Functions: Superconductivity in Boron-Doped Diamond Reexamined. Physical Review Letters, 2007, 98, 047005.	2.9	136
36	Origin of Low Carrier Mobilities in Halide Perovskites. ACS Energy Letters, 2019, 4, 456-463.	8.8	136

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37	One-shot calculation of temperature-dependent optical spectra and phonon-induced band-gap renormalization. Physical Review B, 2016, 94, .	1.1	134
38	Structural and Electronic Properties of Semiconductorâ€Sensitized Solarâ€Cell Interfaces. Advanced Functional Materials, 2011, 21, 4663-4667.	7.8	131
39	Theory of atomic-scale dielectric permittivity at insulator interfaces. Physical Review B, 2005, 71, .	1.1	128
40	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:n band gap of the hybrid organic-inorganic perovskite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>CH</mml:mi><mml:mn>3</mml:mn></mml: Effect of spin-orbit interaction, semicore electrons, an. Physical Review B, 2014, 90, .	1.1	126
41	GW method with the self-consistent Sternheimer equation. Physical Review B, 2010, 81, .	1.1	122
42	Origin of the crossover from polarons to Fermi liquids in transition metal oxides. Nature Communications, 2017, 8, 15769.	5.8	122
43	Phase Diagrams and Stability of Lead-Free Halide Double Perovskites Cs₂BBâ€²X₆: B = Sb and Bi, Bâ€² = Cu, Ag, and Au, and X = Cl, Br, and I. Journal of Physical Chemistry C, 2018, 122, 158-170.	1.5	114
44	The 2021 quantum materials roadmap. JPhys Materials, 2020, 3, 042006.	1.8	111
45	Origin of Superconductivity and Latent Charge Density Wave in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>NbS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></ Physical Review Letters, 2017, 119, 087003.	2.9	108
46	Angle-Resolved Photoemission Spectra of Graphene from First-Principles Calculations. Nano Letters, 2009, 9, 4234-4239.	4.5	102
47	Quantum nuclear dynamics in the photophysics of diamondoids. Nature Communications, 2013, 4, 2006.	5.8	88
48	Raman Spectrum of the Organicâ€“Inorganic Halide Perovskite CH₃NH₃PbI₃ from First Principles and High-Resolution Low-Temperature Raman Measurements. Journal of Physical Chemistry C, 2018, 122, 21703-21717.	1.5	87
49	Stochastic Approach to Phonon-Assisted Optical Absorption. Physical Review Letters, 2015, 115, 177401.	2.9	85
50	Ab initiotheory of polarons: Formalism and applications. Physical Review B, 2019, 99, .	1.1	84
51	Dielectric Discontinuity at Interfaces in the Atomic-Scale Limit: Permittivity of Ultrathin Oxide Films on Silicon. Physical Review Letters, 2003, 91, 267601.	2.9	82
52	Route to Stable Lead-Free Double Perovskites with the Electronic Structure of CH₃NH₃PbI₃: A Case for Mixed-Cation [Cs/CH₃NH₃/CH(NH₂)₂]₂InBiBr₆. Journal of Physical Chemistry Letters, 2017, 8, 3917-3924.	2.1	82
53	Polarons from First Principles, without Supercells. Physical Review Letters, 2019, 122, 246403.	2.9	79
54	Carrier Lifetimes and Polaronic Mass Enhancement in the Hybrid Halide Perovskite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:msub><mml:mrow><mml:mi>CH</mml:mi></mml:mrow><mml:mrow><mml:mn>3</ Physical Review Letters, 2018, 121, 086402.	2.9	76

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55	Hole mobility of strained GaN from first principles. Physical Review B, 2019, 100, .	1.1	75
56	Dimensional Crossover in the Carrier Mobility of Two-Dimensional Semiconductors: The Case of InSe. Nano Letters, 2019, 19, 1774-1781.	4.5	75
57	Graphene-based technologies for energy applications, challenges and perspectives. 2D Materials, 2015, 2, 030204.	2.0	74
58	First-Principles Study of Electron Linewidths in Graphene. Physical Review Letters, 2009, 102, 076803.	2.9	72
59	Two-gap superconductivity in heavily<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>n</mml:mi></mml:math>-doped graphene:Ab initioMigdal-Eliashberg theory. Physical Review B, 2014, 90, .	1.1	71
60	GW quasiparticle bandgaps of anatase TiO₂starting from DFT +U. Journal of Physics Condensed Matter, 2012, 24, 202201.	0.7	67
61	Atomic-Scale Observation of Multiconformational Binding and Energy Level Alignment of Ruthenium-Based Photosensitizers on TiO₂ Anatase. Nano Letters, 2014, 14, 563-569.	4.5	67
62	Ferroelectric Grapheneâ€“Perovskite Interfaces. Journal of Physical Chemistry Letters, 2015, 6, 2496-2502.	2.1	67
63	Electron-phonon interaction and pairing mechanism in superconducting Ca-intercalated bilayer graphene. Scientific Reports, 2016, 6, 21414.	1.6	65
64	Structural and electronic properties of an abrupt<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>4</mml:mn><mml:mi>H</mml:mi><mml:mtext>â^'</mml:mtext><mml:mi>SiC</mml:mi><mml model: Classical molecular dynamics simulations and density functional calculations. Physical Review B, 2007, 76, .	1.5	64
65	Route to High Hole Mobility in GaN via Reversal of Crystal-Field Splitting. Physical Review Letters, 2019, 123, 096602.	2.9	63
66	Ideal Energyâ€Level Alignment at the ZnO/P3HT Photovoltaic Interface. Advanced Functional Materials, 2012, 22, 5089-5095.	7.8	58
67	Band Structures of Plasmonic Polarons. Physical Review Letters, 2015, 114, 146404.	2.9	57
68	Theory of the special displacement method for electronic structure calculations at finite temperature. Physical Review Research, 2020, 2, .	1.3	57
69	Strong Carrier Lifetime Enhancement in GaAs Nanowires Coated with Semiconducting Polymer. Nano Letters, 2012, 12, 6293-6301.	4.5	54
70	Infrared Spectra at Surfaces and Interfaces from First Principles: Evolution of the Spectra across theSi(100)â^'SiO2Interface. Physical Review Letters, 2005, 95, 187402.	2.9	53
71	Ultrafast entangling gates between nuclear spins using photoexcited triplet states. Nature Physics, 2012, 8, 596-600.	6.5	51
72	Van Hove singularity and apparent anisotropy in the electron-phonon interaction in graphene. Physical Review B, 2008, 77, .	1.1	50

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73	Atomistic models of the Si(100)â€“SiO2interface: structural, electronic and dielectric properties. Journal of Physics Condensed Matter, 2005, 17, S2065-S2074.	0.7	48
74	First-principles predictions of Hall and drift mobilities in semiconductors. Physical Review Research, 2021, 3, .	1.3	48
75	Unified theory of electronâ€“phonon renormalization and phonon-assisted optical absorption. Journal of Physics Condensed Matter, 2014, 26, 365503.	0.7	47
76	Electronic and dielectric properties of a suboxide interlayer at the siliconâ€“oxide interface in MOS devices. Surface Science, 2005, 586, 183-191.	0.8	46
77	Surface properties of lead-free halide double perovskites: Possible visible-light photo-catalysts for water splitting. Applied Physics Letters, 2018, 112, .	1.5	46
78	Limits to Electrical Mobility in Lead-Halide Perovskite Semiconductors. Journal of Physical Chemistry Letters, 2021, 12, 3607-3617.	2.1	45
79	Coexistence of Superconductivity with Enhanced Charge Density Wave Order in the Two-Dimensional Limit of TaSe₂. Journal of Physical Chemistry Letters, 2019, 10, 4076-4081.	2.1	44
80	Structural, electronic, elastic, power, and transport properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î²</mml:mi><mml:mtext>â^'</mml:mtext><mml:msub><mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>from first principles. Physical Review Research, 2020, 2, .	1.3	43
81	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">CaBaCo</mml:mi></mml:mrow><mml:mn>4</mml:mn></mml:msub></mml:math><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mn>7</mml:mn></mml:msub></mml:math>: A	1.1	42
82	Structure of a Water Monolayer on the Anatase<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>TiO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub><mml:mo stretchy="false">(</mml:mo><mml:mn>101</mml:mn><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 367 Td (stretchy="false">)</mml:mo>	1.5	42
83	Monolayer 1T-NbSe ₂ as a 2D-correlated magnetic insulator. Science Advances, 2021, 7, eabi6339.	4.7	39
84	Ab initioSternheimer-GW method for quasiparticle calculations using plane waves. Physical Review B, 2013, 88, .	1.1	36
85	Theory of electron-plasmon coupling in semiconductors. Physical Review B, 2016, 94, .	1.1	36
86	On the combined use of GW approximation and cumulant expansion in the calculations of quasiparticle spectra: The paradigm of Si valence bands. Physical Review B, 2016, 94, .	1.1	36
87	Nonadiabatic Kohn Anomaly in Heavily Boron-Doped Diamond. Physical Review Letters, 2017, 119, 017001.	2.9	36
88	Oxide Analogs of Halide Perovskites and the New Semiconductor Ba₂AgIO₆. Journal of Physical Chemistry Letters, 2019, 10, 1722-1728.	2.1	36
89	First-principles study of superconductivity and Fermi-surface nesting in ultrahard transition metal carbides. Physical Review B, 2008, 77, .	1.1	32
90	Ruddlesdenâ€“Popperâ€Phase Hybrid Halide Perovskite/Smallâ€Molecule Organic Blend Memory Transistors. Advanced Materials, 2021, 33, e2003137.	11.1	32

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91	Crossover from lattice to plasmonic polarons of a spin-polarised electron gas in ferromagnetic EuO. Nature Communications, 2018, 9, 2305.	5.8	31
92	Excitons in one-dimensional van der Waals materials:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Sb</mml:mi><mml:mn>2</mml:mn></mml: mathvariant="normal">S</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>nanoribbons. Physical Review B, 2015, 92, .	1.1	30
93	Phonon-Limited Mobility and Electronâ€“Phonon Coupling in Lead-Free Halide Double Perovskites. Journal of Physical Chemistry Letters, 2021, 12, 4474-4482.	2.1	30
94	Origin of superconductivity in boron-doped silicon carbide from first principles. Physical Review B, 2009, 79, .	1.1	27
95	Single-Molecule Vibrational Spectroscopy of H₂O on Anatase TiO₂(101). Journal of Physical Chemistry C, 2017, 121, 1182-1187.	1.5	27
96	Electron-plasmon and electron-phonon satellites in the angle-resolved photoelectron spectra of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>n</mml:mi></mml:math> -doped anatase <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml: Physical Review B, 2018, 97, .	1.1	27
97	Dielectric effect of a thin SiO2 interlayer at the interface between silicon and high-k oxides. Microelectronic Engineering, 2004, 72, 299-303.	1.1	26
98	Quantitative Analysis of Valence Photoemission Spectra and Quasiparticle Excitations at Chromophore-Semiconductor Interfaces. Physical Review Letters, 2012, 109, 116801.	2.9	26
99	Intrinsic quantum confinement in formamidinium lead triiodide perovskite. Nature Materials, 2020, 19, 1201-1206.	13.3	26
100	Universal Scaling of Intrinsic Resistivity in Twoâ€Dimensional Metallic Borophene. Angewandte Chemie - International Edition, 2018, 57, 4585-4589.	7.2	25
101	Ab initio calculation of spin fluctuation spectra using time-dependent density functional perturbation theory, plane waves, and pseudopotentials. Physical Review B, 2018, 97, .	1.1	25
102	O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>1</mml:mn><mml:mi>s</mml:mi></mml:mrow></mml:math>core-level shifts at the anatase TiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>(101)/N3 photovoltaic interface: Signature of H-bonded supramolecular assembly. Physical Review B, 2011, 84, .	1.1	24
103	Spectral fingerprints of electron-plasmon coupling. Physical Review B, 2015, 92, .	1.1	24
104	Van der Waals Interactions and Anharmonicity in the Lattice Vibrations, Dielectric Constants, Effective Charges, and Infrared Spectra of the Organicâ€“Inorganic Halide Perovskite CH₃NH₃PbI₃. Journal of Physical Chemistry C, 2017, 121, 18459-18471.	1.5	24
105	Abrupt model interface for the 4H(1000)SiC-SiO2 interface. Microelectronic Engineering, 2005, 80, 38-41.	1.1	23
106	Equivalent oxide thickness of a thin oxide interlayer in gate insulator stacks on silicon. Applied Physics Letters, 2005, 86, 192901.	1.5	23
107	Graphene Oxide/Perovskite Interfaces For Photovoltaics. Journal of Physical Chemistry C, 2018, 122, 16715-16726.	1.5	22
108	Proton-Induced Fixed Positive Charge at the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Si</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mn>100</mml:mn><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 62 Td (stretchy="false">)</mml mathvariant="normal">â^'</mml:mtext><mml:msub><mml:mi>SiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>Interfac Physical Review Letters, 2007, 99, 126102.	2.9	21

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109	Mixed Wannier-Bloch Functions for Electrons and Phonons in Periodic Systems. Physical Review Letters, 2006, 96, 216403.	2.9	20
110	The GW plus cumulant method and plasmonic polarons: application to the homogeneous electron gas*. European Physical Journal B, 2016, 89, 1.	0.6	20
111	Highâ€Efficiency Fullerene Solar Cells Enabled by a Spontaneously Formed Mesostructured CuSCNâ€Nanowire Heterointerface. Advanced Science, 2018, 5, 1700980.	5.6	19
112	Electron-polaron dichotomy of charge carriers in perovskite oxides. Communications Physics, 2020, 3, .	2.0	19
113	Crystallographic, Optical, and Electronic Properties of the Cs2AgBi1â€“xInxBr6 Double Perovskite: Understanding the Fundamental Photovoltaic Efficiency Challenges. ACS Energy Letters, 2021, 6, 1073-1081.	8.8	19
114	Modeling of Si 2p core-level shifts at Siâ€“(ZrO2)x(SiO2)1â^'x interfaces. Applied Physics Letters, 2002, 81, 4233-4235.	1.5	18
115	Theory of Electromagnons in CuO. Physical Review Letters, 2015, 114, 197201.	2.9	18
116	Atomic Structure of Water Monolayer on Anatase TiO₂(101) Surface. Journal of Physical Chemistry C, 2018, 122, 11954-11960.	1.5	18
117	Manipulating surface magnetic order in iron telluride. Science Advances, 2019, 5, eaav3478.	4.7	18
118	Efficient First-Principles Methodology for the Calculation of the All-Phonon Inelastic Scattering in Solids. Physical Review Letters, 2021, 127, 207401.	2.9	18
119	Entangling Remote Nuclear Spins Linked by a Chromophore. Physical Review Letters, 2010, 104, 200501.	2.9	17
120	Many-body renormalization of the electron effective mass of InSe. Physical Review B, 2020, 101, .	1.1	16
121	Multiphonon diffuse scattering in solids from first principles: Application to layered crystals and two-dimensional materials. Physical Review B, 2021, 104, .	1.1	16
122	Role of Fluorine in the Iron Pnictides: Phonon Softening and Effective Hole Doping. Physical Review Letters, 2009, 102, 147003.	2.9	15
123	Time-dependent density functional theory using atomic orbitals and the self-consistent Sternheimer equation. Physical Review B, 2014, 89, .	1.1	15
124	Interfaces Between Grapheneâ€Related Materials and MAPbI 3 : Insights from Firstâ€Principles. Advanced Materials Interfaces, 2018, 5, 1800496.	1.9	15
125	Quasiparticle<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mm structures and Fermi surfaces of bulk and monolayer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>NbS</mml:mi><mml:mn>2</mml:mn></mml:msub></m Physical Review B, 2018, 98, .	1.1	15
126	Dynamic Rashba-Dresselhaus Effect. Physical Review Letters, 2021, 127, 237601.	2.9	15

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127	Linear optical response of finite systems using multishift linear system solvers. Journal of Chemical Physics, 2014, 141, 044117.	1.2	14
128	First-principles study of structurally modulated multiferroic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mtext>CaMn</mml:mtext><mml:mn>1</mml:mn> Physical Review B, 2015, 91, .	1.1	14
129	Slot-Die-Printed Two-Dimensional ZrS₃ Charge Transport Layer for Perovskite Light-Emitting Diodes. ACS Applied Materials & Interfaces, 2019, 11, 48021-48028.	4.0	13
130	Theory and Computation of Hall Scattering Factor in Graphene. Nano Letters, 2020, 20, 8861-8865.	4.5	13
131	First-principles study of electron transport in ScN. Physical Review B, 2021, 104, .	1.1	13
132	Quasiparticle Band Structure and Phonon-Induced Band Gap Renormalization of the Lead-Free Halide Double Perovskite Cs₂InAgCl₆. Journal of Physical Chemistry C, 2021, 125, 21689-21700.	1.5	13
133	CeTaN₃ and CeNbN₃: Prospective Nitride Perovskites with Optimal Photovoltaic Band Gaps. Chemistry of Materials, 2022, 34, 2107-2122.	3.2	13
134	Dielectric screening in extended systems using the self-consistent Sternheimer equation and localized basis sets. Physical Review B, 2012, 85, .	1.1	12
135	SternheimerGW: A program for calculating <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e1442" altimg="si24.svg"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math> quasiparticle band structures and spectral functions without unoccupied states. Computer Physics Communications, 2020, 247, 106856.	3.0	12
136	GW band structure of monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>MoS</mml:mi></mml:mrow><mml:mn>2</mml:mn> using the SternheimerGW method and effect of dielectric environment. Physical Review B, 2021, 103, .	1.1	11
137	Dose and dose-rate effects on NPN bipolar junction transistors irradiated at high temperature. IEEE Transactions on Nuclear Science, 2002, 49, 1474-1479.	1.2	10
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