

Feliciano Giustino

List of Publications by Year in descending order

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174
papers

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17440

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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.	1.8	4,303
2	Perovskite-perovskite tandem photovoltaics with optimized band gaps. Science, 2016, 354, 861-865.	12.6	1,107
3	Electron-phonon interactions from first principles. Reviews of Modern Physics, 2017, 89, .	45.6	947
4	Electron-phonon coupling in hybrid lead halide perovskites. Nature Communications, 2016, 7, .	12.8	919
5	Toward Lead-Free Perovskite Solar Cells. ACS Energy Letters, 2016, 1, 1233-1240.	17.4	848
6	Steric engineering of metal-halide perovskites with tunable optical band gaps. Nature Communications, 2014, 5, 5757.	12.8	787
7	EPW: Electron-phonon coupling, transport and superconducting properties using maximally localized Wannier functions. Computer Physics Communications, 2016, 209, 116-133.	7.5	777
8	Lead-Free Halide Double Perovskites via Heterovalent Substitution of Noble Metals. Journal of Physical Chemistry Letters, 2016, 7, 1254-1259.	4.6	761
9	Cs ₂ InAgCl ₆ : A New Lead-Free Halide Double Perovskite with Direct Band Gap. Journal of Physical Chemistry Letters, 2017, 8, 772-778.	4.6	752
10	Electron-phonon interaction using Wannier functions. Physical Review B, 2007, 76, .	3.2	625
11	TiO ₂ Anatase with a Bandgap in the Visible Region. Nano Letters, 2014, 14, 6533-6538.	9.1	531
12	Band Gaps of the Lead-Free Halide Double Perovskites Cs ₂ BiAgCl ₆ and Cs ₂ BiAgBr ₆ from Theory and Experiment. Journal of Physical Chemistry Letters, 2016, 7, 2579-2585.	4.6	529
13	Cubic or Orthorhombic? Revealing the Crystal Structure of Metastable Black-Phase CsPbI ₃ by Theory and Experiment. ACS Energy Letters, 2018, 3, 1787-1794.	17.4	455
14	Oxygen redox chemistry without excess alkali-metal ions in Na _{2/3} [Mg _{0.28} Mn _{0.72}]O ₂ . Nature Chemistry, 2018, 10, 288-295.	13.6	414
15	Dislocation-Driven Deformations in Graphene. Science, 2012, 337, 209-212.	12.6	332
16	EPW: A program for calculating the electron-phonon coupling using maximally localized Wannier functions. Computer Physics Communications, 2010, 181, 2140-2148.	7.5	324
17	Vibrational Properties of the Organic-Inorganic Halide Perovskite CH ₃ NH ₃ PbI ₃ from Theory and Experiment: Factor Group Analysis, First-Principles Calculations, and Low-Temperature Infrared Spectra. Journal of Physical Chemistry C, 2015, 119, 25703-25718.	3.1	276
18	Confinement Effects in Low-Dimensional Lead Iodide Perovskite Hybrids. Chemistry of Materials, 2016, 28, 4554-4562.	6.7	263

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19	Bimolecular recombination in methylammonium lead triiodide perovskite is an inverse absorption process. <i>Nature Communications</i> , 2018, 9, 293.	12.8	243
20	Electron-Phonon Renormalization of the Direct Band Gap of Diamond. <i>Physical Review Letters</i> , 2010, 105, 265501.	7.8	241
21	Fröhlich Electron-Phonon Vertex from First Principles. <i>Physical Review Letters</i> , 2015, 115, 176401.	7.8	232
22	Towards predictive many-body calculations of phonon-limited carrier mobilities in semiconductors. <i>Physical Review B</i> , 2018, 97, .	3.2	224
23	Anisotropic Migdal-Eliashberg theory using Wannier functions. <i>Physical Review B</i> , 2013, 87, .	3.2	220
24	Computational Screening of Homovalent Lead Substitution in Organic-Inorganic Halide Perovskites. <i>Journal of Physical Chemistry C</i> , 2016, 120, 166-173.	3.1	208
25	Solution-Processed Cesium Hexabromopalladate(IV), Cs ₂ PdBr ₆ , for Optoelectronic Applications. <i>Journal of the American Chemical Society</i> , 2017, 139, 6030-6033.	13.7	189
26	Velocity Renormalization and Carrier Lifetime in Graphene from the Electron-Phonon Interaction. <i>Physical Review Letters</i> , 2007, 99, 086804.	7.8	183
27	First-Principles Prediction of Doped Graphane as a High-Temperature Electron-Phonon Superconductor. <i>Physical Review Letters</i> , 2010, 105, 037002.	7.8	178
28	$\langle G \cdot W \rangle$ quasiparticle band structures of stibnite, antimonselite, bismuthinite, and guanajuatite. <i>Physical Review B</i> , 2013, 87, .	8.2	178
29	First-principles calculations of charge carrier mobility and conductivity in bulk semiconductors and two-dimensional materials. <i>Reports on Progress in Physics</i> , 2020, 83, 036501.	20.1	176
30	Small phonon contribution to the photoemission kink in the copper oxide superconductors. <i>Nature</i> , 2008, 452, 975-978.	27.8	157
31	Electron-Phonon Interactions in Graphene, Bilayer Graphene, and Graphite. <i>Nano Letters</i> , 2008, 8, 4229-4233.	9.1	156
32	Band Offsets at the Si ₂ SiO ₂ interface from Many-Body Perturbation Theory. <i>Physical Review Letters</i> , 2008, 100, 186401.	15.1	151
33	<i>i>GW</i> Band Structures and Carrier Effective Masses of CH₃NH₃PbI₃ and Hypothetical Perovskites of the Type APbI₃: A = NH₄, PH₄, AsH₄, and SbH₄. <i>Journal of Physical Chemistry C</i>, 2015, 119, 25209-25219.</i>	3.1	144
34	The geometric blueprint of perovskites. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 5397-5402.	7.1	138
35	Electron-Phonon Interaction via Electronic and Lattice Wannier Functions: Superconductivity in Boron-Doped Diamond Reexamined. <i>Physical Review Letters</i> , 2007, 98, 047005.	7.8	136
36	Origin of Low Carrier Mobilities in Halide Perovskites. <i>ACS Energy Letters</i> , 2019, 4, 456-463.	17.4	136

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37	One-shot calculation of temperature-dependent optical spectra and phonon-induced band-gap renormalization. <i>Physical Review B</i> , 2016, 94, .	3.2	134
38	Structural and Electronic Properties of Semiconductor-Sensitized Solar-Cell Interfaces. <i>Advanced Functional Materials</i> , 2011, 21, 4663-4667.	14.9	131
39	Theory of atomic-scale dielectric permittivity at insulator interfaces. <i>Physical Review B</i> , 2005, 71, .	3.2	128
40	band gap of the hybrid organic-inorganic perovskite $\text{CH}_3\text{NH}_3\text{PbI}_3$ Effect of spin-orbit interaction, semicore electrons, an. <i>Physical Review B</i> , 2014, 90, .	3.2	126
41	CW method with the self-consistent Sternheimer equation. <i>Physical Review B</i> , 2010, 81, .	3.2	122
42	Origin of the crossover from polarons to Fermi liquids in transition metal oxides. <i>Nature Communications</i> , 2017, 8, 15769.	12.8	122
43	Phase Diagrams and Stability of Lead-Free Halide Double Perovskites $\text{Cs}_2\text{BB}_2\text{X}_6$: B = Sb and Bi, B^{2+} = Cu, Ag, and Au, and X = Cl, Br, and I. <i>Journal of Physical Chemistry C</i> , 2018, 122, 158-170.	3.1	114
44	The 2021 quantum materials roadmap. <i>JPhys Materials</i> , 2020, 3, 042006.	4.2	111
45	Origin of Superconductivity and Latent Charge Density Wave in NbS_2 <i>Physical Review Letters</i> , 2017, 119, 087003.	7.8	108
46	Angle-Resolved Photoemission Spectra of Graphene from First-Principles Calculations. <i>Nano Letters</i> , 2009, 9, 4234-4239.	9.1	102
47	Quantum nuclear dynamics in the photophysics of diamondoids. <i>Nature Communications</i> , 2013, 4, 2006.	12.8	88
48	Raman Spectrum of the Organic-Inorganic Halide Perovskite $\text{CH}_3\text{NH}_3\text{PbI}_3$ from First Principles and High-Resolution Low-Temperature Raman Measurements. <i>Journal of Physical Chemistry C</i> , 2018, 122, 21703-21717.	3.1	87
49	Stochastic Approach to Phonon-Assisted Optical Absorption. <i>Physical Review Letters</i> , 2015, 115, 177401.	7.8	85
50	<i>Ab initio</i> theory of polarons: Formalism and applications. <i>Physical Review B</i> , 2019, 99, .	3.2	84
51	Dielectric Discontinuity at Interfaces in the Atomic-Scale Limit: Permittivity of Ultrathin Oxide Films on Silicon. <i>Physical Review Letters</i> , 2003, 91, 267601.	7.8	82
52	Route to Stable Lead-Free Double Perovskites with the Electronic Structure of $\text{CH}_3\text{NH}_3\text{PbI}_3$: A Case for Mixed-Cation $[\text{Cs}/\text{CH}_3\text{NH}_3]/\text{CH}(\text{NH}_2)_2$ InBiBr_6 . <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3917-3924.	4.6	82
53	Polarons from First Principles, without Supercells. <i>Physical Review Letters</i> , 2019, 122, 246403.	7.8	79
54	Carrier Lifetimes and Polaronic Mass Enhancement in the Hybrid Halide Perovskite $\text{CH}_3\text{NH}_3\text{PbI}_3$ <i>Physical Review Letters</i> , 2018, 121, 086402.	7.8	76

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55	Hole mobility of strained GaN from first principles. <i>Physical Review B</i> , 2019, 100, .	3.2	75
56	Dimensional Crossover in the Carrier Mobility of Two-Dimensional Semiconductors: The Case of InSe. <i>Nano Letters</i> , 2019, 19, 1774-1781.	9.1	75
57	Graphene-based technologies for energy applications, challenges and perspectives. <i>2D Materials</i> , 2015, 2, 030204.	4.4	74
58	First-Principles Study of Electron Linewidths in Graphene. <i>Physical Review Letters</i> , 2009, 102, 076803.	7.8	72
59	Two-gap superconductivity in heavily n -doped graphene: Ab initio Migdal-Eliashberg theory. <i>Physical Review B</i> , 2014, 90, .	3.2	71
60	GW quasiparticle bandgaps of anatase TiO_2 starting from DFT + U . <i>Journal of Physics Condensed Matter</i> , 2012, 24, 202201.	1.8	67
61	Atomic-Scale Observation of Multiconformational Binding and Energy Level Alignment of Ruthenium-Based Photosensitizers on TiO_2 Anatase. <i>Nano Letters</i> , 2014, 14, 563-569.	9.1	67
62	Ferroelectric Graphene-Perovskite Interfaces. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 2496-2502.	4.6	67
63	Electron-phonon interaction and pairing mechanism in superconducting Ca-intercalated bilayer graphene. <i>Scientific Reports</i> , 2016, 6, 21414.	3.3	65
64	Structural and electronic properties of an abrupt 4H -SiC model: Classical molecular dynamics simulations and density functional calculations. <i>Physical Review B</i> , 2007, 76, .	3.5	64
65	Route to High Hole Mobility in GaN via Reversal of Crystal-Field Splitting. <i>Physical Review Letters</i> , 2019, 123, 096602.	7.8	63
66	Ideal Energy Level Alignment at the ZnO/P3HT Photovoltaic Interface. <i>Advanced Functional Materials</i> , 2012, 22, 5089-5095.	14.9	58
67	Band Structures of Plasmonic Polarons. <i>Physical Review Letters</i> , 2015, 114, 146404.	7.8	57
68	Theory of the special displacement method for electronic structure calculations at finite temperature. <i>Physical Review Research</i> , 2020, 2, .	3.6	57
69	Strong Carrier Lifetime Enhancement in GaAs Nanowires Coated with Semiconducting Polymer. <i>Nano Letters</i> , 2012, 12, 6293-6301.	9.1	54
70	Infrared Spectra at Surfaces and Interfaces from First Principles: Evolution of the Spectra across the $\text{Si}(100)\text{-SiO}_2$ Interface. <i>Physical Review Letters</i> , 2005, 95, 187402.	7.8	53
71	Ultrafast entangling gates between nuclear spins using photoexcited triplet states. <i>Nature Physics</i> , 2012, 8, 596-600.	16.7	51
72	Van Hove singularity and apparent anisotropy in the electron-phonon interaction in graphene. <i>Physical Review B</i> , 2008, 77, .	3.2	50

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73	Atomistic models of the Si(100)–SiO ₂ interface: structural, electronic and dielectric properties. Journal of Physics Condensed Matter, 2005, 17, S2065-S2074.	1.8	48
74	First-principles predictions of Hall and drift mobilities in semiconductors. Physical Review Research, 2021, 3, .	3.6	48
75	Unified theory of electron–phonon renormalization and phonon-assisted optical absorption. Journal of Physics Condensed Matter, 2014, 26, 365503.	1.8	47
76	Electronic and dielectric properties of a suboxide interlayer at the silicon–oxide interface in MOS devices. Surface Science, 2005, 586, 183-191.	1.9	46
77	Surface properties of lead-free halide double perovskites: Possible visible-light photo-catalysts for water splitting. Applied Physics Letters, 2018, 112, .	3.3	46
78	Limits to Electrical Mobility in Lead-Halide Perovskite Semiconductors. Journal of Physical Chemistry Letters, 2021, 12, 3607-3617.	4.6	45
79	Coexistence of Superconductivity with Enhanced Charge Density Wave Order in the Two-Dimensional Limit of TaSe ₂ . Journal of Physical Chemistry Letters, 2019, 10, 4076-4081.	4.6	44
80	Structural, electronic, elastic, power, and transport properties of $\text{O}^{\wedge 2}$ from first principles. Physical Review Research, 2020, 2, .	3.6	43
81	Structure of a Water Monolayer on the Anatase $\text{CaBaCo}_4\text{O}_7$: A	3.2	42
82	Structure of a Water Monolayer on the Anatase TiO_2 (101) Surface. Physical Review Letters, 2012, 108, 017201.	3.1	42
83	Monolayer 1T-NbSe ₂ as a 2D-correlated magnetic insulator. Science Advances, 2021, 7, eabi6339.	10.3	39
84	<i>Ab initio</i> Sternheimer-GW method for quasiparticle calculations using plane waves. Physical Review B, 2013, 88, .	3.2	36
85	Theory of electron-plasmon coupling in semiconductors. Physical Review B, 2016, 94, .	3.2	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, .	3.2	36
87	Nonadiabatic Kohn Anomaly in Heavily Boron-Doped Diamond. Physical Review Letters, 2017, 119, 017001.	7.8	36
88	Oxide Analogs of Halide Perovskites and the New Semiconductor Ba ₂ AgIO ₆ . Journal of Physical Chemistry Letters, 2019, 10, 1722-1728.	4.6	36
89	First-principles study of superconductivity and Fermi-surface nesting in ultrahard transition metal carbides. Physical Review B, 2008, 77, .	3.2	32
90	Ruddlesden–Popper Phase Hybrid Halide Perovskite/Small Molecule Organic Blend Memory Transistors. Advanced Materials, 2021, 33, e2003137.	21.0	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.	12.8	31
92	Excitons in one-dimensional van der Waals materials: S_3 nanoribbons. Physical Review B, 2015, 92, .	3.2	30
93	Phonon-Limited Mobility and Electron-Phonon Coupling in Lead-Free Halide Double Perovskites. Journal of Physical Chemistry Letters, 2021, 12, 4474-4482.	4.6	30
94	Origin of superconductivity in boron-doped silicon carbide from first principles. Physical Review B, 2009, 79, .	3.2	27
95	Single-Molecule Vibrational Spectroscopy of H_2O on Anatase $TiO_2(101)$. Journal of Physical Chemistry C, 2017, 121, 1182-1187.	3.1	27
96	Electron-plasmon and electron-phonon satellites in the angle-resolved photoelectron spectra of n-doped anatase TiO_2 . Physical Review B, 2018, 97, .	3.2	27
97	Dielectric effect of a thin SiO_2 interlayer at the interface between silicon and high-k oxides. Microelectronic Engineering, 2004, 72, 299-303.	2.4	26
98	Quantitative Analysis of Valence Photoemission Spectra and Quasiparticle Excitations at Chromophore-Semiconductor Interfaces. Physical Review Letters, 2012, 109, 116801.	7.8	26
99	Intrinsic quantum confinement in formamidinium lead triiodide perovskite. Nature Materials, 2020, 19, 1201-1206.	27.5	26
100	Universal Scaling of Intrinsic Resistivity in Two-Dimensional Metallic Borophene. Angewandte Chemie - International Edition, 2018, 57, 4585-4589.	13.8	25
101	<i>Ab initio</i> calculation of spin fluctuation spectra using time-dependent density functional perturbation theory, plane waves, and pseudopotentials. Physical Review B, 2018, 97, .	3.2	25
102	$1s$ core-level shifts at the anatase $TiO_2(101)/N_3$ photovoltaic interface: Signature of H-bonded supramolecular assembly. Physical Review B, 2011, 84, .	3.2	24
103	Spectral fingerprints of electron-plasmon coupling. Physical Review B, 2015, 92, .	3.2	24
104	Van der Waals Interactions and Anharmonicity in the Lattice Vibrations, Dielectric Constants, Effective Charges, and Infrared Spectra of the Organic-Inorganic Halide Perovskite $CH_3NH_3PbI_3$. Journal of Physical Chemistry C, 2017, 121, 18459-18471.	3.1	24
105	Abrupt model interface for the $4H(100)SiC-SiO_2$ interface. Microelectronic Engineering, 2005, 80, 38-41.	2.4	23
106	Equivalent oxide thickness of a thin oxide interlayer in gate insulator stacks on silicon. Applied Physics Letters, 2005, 86, 192901.	3.3	23
107	Graphene Oxide/Perovskite Interfaces For Photovoltaics. Journal of Physical Chemistry C, 2018, 122, 16715-16726.	3.1	22
108	Proton-Induced Fixed Positive Charge at the SiO_2 Interface. Physical Review Letters, 2007, 99, 126102.	7.8	21

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109	Mixed Wannier-Bloch Functions for Electrons and Phonons in Periodic Systems. <i>Physical Review Letters</i> , 2006, 96, 216403.	7.8	20
110	The GW plus cumulant method and plasmonic polarons: application to the homogeneous electron gas*. <i>European Physical Journal B</i> , 2016, 89, 1.	1.5	20
111	High-Efficiency Fullerene Solar Cells Enabled by a Spontaneously Formed Mesostructured CuSCN-Nanowire Heterointerface. <i>Advanced Science</i> , 2018, 5, 1700980.	11.2	19
112	Electron-polaron dichotomy of charge carriers in perovskite oxides. <i>Communications Physics</i> , 2020, 3, .	5.3	19
113	Crystallographic, Optical, and Electronic Properties of the Cs ₂ AgBi _{1-x} In _x Br ₆ Double Perovskite: Understanding the Fundamental Photovoltaic Efficiency Challenges. <i>ACS Energy Letters</i> , 2021, 6, 1073-1081.	17.4	19
114	Modeling of Si 2p core-level shifts at Si-(ZrO ₂) _x (SiO ₂) _{1-x} interfaces. <i>Applied Physics Letters</i> , 2002, 81, 4233-4235.	3.3	18
115	Theory of Electromagnons in CuO. <i>Physical Review Letters</i> , 2015, 114, 197201.	7.8	18
116	Atomic Structure of Water Monolayer on Anatase TiO ₂ (101) Surface. <i>Journal of Physical Chemistry C</i> , 2018, 122, 11954-11960.	3.1	18
117	Manipulating surface magnetic order in iron telluride. <i>Science Advances</i> , 2019, 5, eaav3478.	10.3	18
118	Efficient First-Principles Methodology for the Calculation of the All-Phonon Inelastic Scattering in Solids. <i>Physical Review Letters</i> , 2021, 127, 207401.	7.8	18
119	Entangling Remote Nuclear Spins Linked by a Chromophore. <i>Physical Review Letters</i> , 2010, 104, 200501.	7.8	17
120	Many-body renormalization of the electron effective mass of InSe. <i>Physical Review B</i> , 2020, 101, .	3.2	16
121	Multiphonon diffuse scattering in solids from first principles: Application to layered crystals and two-dimensional materials. <i>Physical Review B</i> , 2021, 104, .	3.2	16
122	Role of Fluorine in the Iron Pnictides: Phonon Softening and Effective Hole Doping. <i>Physical Review Letters</i> , 2009, 102, 147003.	7.8	15
123	Time-dependent density functional theory using atomic orbitals and the self-consistent Sternheimer equation. <i>Physical Review B</i> , 2014, 89, .	3.2	15
124	Interfaces Between Graphene-Related Materials and MAPbI ₃ : Insights from First-Principles. <i>Advanced Materials Interfaces</i> , 2018, 5, 1800496.	3.7	15
125	Quasiparticle structures and Fermi surfaces of bulk and monolayer NbS ₂ . <i>Physical Review B</i> , 2018, 98, .	3.2	15
126	Dynamic Rashba-Dresselhaus Effect. <i>Physical Review Letters</i> , 2021, 127, 237601.	7.8	15

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127	Linear optical response of finite systems using multishift linear system solvers. Journal of Chemical Physics, 2014, 141, 044117.	3.0	14
128	First-principles study of structurally modulated multiferroic CaMn_2O_7 . Physical Review B, 2015, 91, .	3.2	14
129	Slot-Die-Printed Two-Dimensional ZrS_3 Charge Transport Layer for Perovskite Light-Emitting Diodes. ACS Applied Materials & Interfaces, 2019, 11, 48021-48028.	8.0	13
130	Theory and Computation of Hall Scattering Factor in Graphene. Nano Letters, 2020, 20, 8861-8865.	9.1	13
131	First-principles study of electron transport in ScN. Physical Review B, 2021, 104, .	3.2	13
132	Quasiparticle Band Structure and Phonon-Induced Band Gap Renormalization of the Lead-Free Halide Double Perovskite $\text{Cs}_2\text{InAgCl}_6$. Journal of Physical Chemistry C, 2021, 125, 21689-21700.	3.1	13
133	CeTa_3 and CeNb_3 : Prospective Nitride Perovskites with Optimal Photovoltaic Band Gaps. Chemistry of Materials, 2022, 34, 2107-2122.	6.7	13
134	Dielectric screening in extended systems using the self-consistent Sternheimer equation and localized basis sets. Physical Review B, 2012, 85, .	3.2	12
135	SternheimerGW: A program for calculating quasiparticle band structures and spectral functions without unoccupied states. Computer Physics Communications, 2020, 247, 106856.	7.5	12
136	GW band structure of monolayer MoS_2 using the SternheimerGW method and effect of dielectric environment. Physical Review B, 2021, 103, .	3.2	12
137	Dose and dose-rate effects on NPN bipolar junction transistors irradiated at high temperature. IEEE Transactions on Nuclear Science, 2002, 49, 1474-1479.	2.0	10
138	First-principles study of multiferroic RbFe_2O_7 . Physical Review B, 2014, 90, .	3.2	10
139	Spin waves in metallic iron and nickel measured by soft x-ray resonant inelastic scattering. Physical Review B, 2020, 102, .	3.2	10
140	Superconducting properties of MoTe_2 from <i>ab initio</i> anisotropic Migdal-Eliashberg theory. Physical Review B, 2020, 101, .	3.2	10
141	Unified <i>ab initio</i> description of Fröhlich electron-phonon interactions in two-dimensional and three-dimensional materials. Physical Review B, 2022, 105, .	3.2	10
142	First-principles investigation of hyperfine interactions for nuclear spin entanglement in photoexcited fullerenes. Physical Review B, 2012, 85, .	3.2	9
143	Energy-level alignment and open-circuit voltage at graphene/polymer interfaces: theory and experiment. 2D Materials, 2016, 3, 015003.	4.4	9
144	Exciton-Phonon Interactions in Monolayer Germanium Selenide from First Principles. Journal of Physical Chemistry Letters, 2021, 12, 3802-3808.	4.6	9

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145	Origin of the High Specific Capacity in Sodium Manganese Hexacyanomanganate. Chemistry of Materials, 2022, 34, 4336-4343.	6.7	9
146	Intrinsic and doping-enhanced superconductivity in monolayer H^{I} : Critical role of charge ordering and spin-orbit coupling. Physical Review B, 2022, 105, .		
147	Electronic Structure and Electron-Transport Properties of Three Metal Hexacyanoferrates. Chemistry of Materials, 2021, 33, 7067-7074.	6.7	8
148	Infrared properties of ultrathin oxides on Si(100). Microelectronic Engineering, 2005, 80, 420-423.	2.4	7
149	Publisher's Note: First-Principles Prediction of Doped Graphane as a High-Temperature Electron-Phonon Superconductor [Phys. Rev. Lett. 105 (2010)]. Physical Review Letters, 2010, 105, .	7.8	7
150	Performance of local orbital basis sets in the self-consistent Sternheimer method for dielectric matrices of extended systems. European Physical Journal B, 2012, 85, 1.	1.5	7
151	Inelastic carrier lifetime in bilayer graphene. Applied Physics Letters, 2012, 100, .	3.3	7
152	Electronic Structure at Realistic Si(100)-SiO ₂ Interfaces. Japanese Journal of Applied Physics, 2004, 43, 7895-7898.	1.5	6
153	First-principles theory of infrared absorption spectra at surfaces and interfaces: Application to the Si(100):H ₂ O surface. Physical Review B, 2008, 78, .	3.2	6
154	Hybrid Halide Perovskites: Fundamental Theory and Materials Design. , 2018, , 1-30.		5
155	Model for high-temperature radiation effects in n-p-n bipolar-junction transistors. IEEE Transactions on Nuclear Science, 2002, 49, 2990-2997.	2.0	4
156	Universal Scaling of Intrinsic Resistivity in Two-Dimensional Metallic Borophene. Angewandte Chemie, 2018, 130, 4675-4679.	2.0	4
157	Ultrafast photo-induced phonon hardening due to Pauli blocking in MAPbI ₃ single-crystal and polycrystalline perovskites. JPhys Materials, 2021, 4, 044017.	4.2	4
158	Many-body Green's function approaches to the doped Fröhlich solid: Exact solutions and anomalous mass enhancement. Physical Review B, 2022, 105, .	3.2	4
159	Trellises of Molecular Oxygen on Anatase TiO ₂ (101). Journal of Physical Chemistry C, 2019, 123, 26170-26177.	3.1	2
160	Hybrid Halide Perovskites: Fundamental Theory and Materials Design. , 2020, , 295-324.		2
161	Anisotropic-strain-enhanced hole mobility in GaN by lattice matching to ZnGeN ₂ and MgSiN ₂ . Applied Physics Letters, 2022, 120, .	3.3	2
162	Dose and dose rate effects on NPN bipolar junction transistors irradiated at high temperature. , 0, , .		1

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163	Atomistic model of the 4H(0001)SiC-SiO ₂ interface: structural and electronic properties. AIP Conference Proceedings, 2007, , .	0.4	1
164	Publisher's Note: Role of Fluorine in the Iron Pnictides: Phonon Softening and Effective Hole Doping [Phys. Rev. Lett. 102 (2009)]. Physical Review Letters, 2009, 102, .	7.8	1
165	Solar Cells: Structural and Electronic Properties of Semiconductor-Sensitized Solar-Cell Interfaces (Adv. Funct. Mater. 24/2011). Advanced Functional Materials, 2011, 21, 4798-4798.	14.9	1
166	Modeling the role of the fluorine dopant in the magnetic phase diagram of LaFeAsO _{1-x} F _x superconductors. Physical Review B, 2012, 85, .	3.2	1
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