Claudia Draxl

List of Publications by Year
in descending order

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254	15,009	22099	20307
papers	citations	59 h-index	116 g-index

258	258	258	15163
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Linear optical properties of solids within the full-potential linearized augmented planewave method. Computer Physics Communications, 2006, 175, 1-14.	3.0	1,215
2	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
3	Transport coefficients from first-principles calculations. Physical Review B, 2003, 68, .	1.1	663
4	Big Data of Materials Science: Critical Role of the Descriptor. Physical Review Letters, 2015, 114, 105503.	2.9	658
5	Band-structure topologies of graphene: Spin-orbit coupling effects from first principles. Physical Review B, 2009, 80, .	1.1	579
6	Optical Constants and Inelastic Electron-Scattering Data for 17 Elemental Metals. Journal of Physical and Chemical Reference Data, 2009, 38, 1013-1092.	1.9	487
7	ElaStic: A tool for calculating second-order elastic constants from first principles. Computer Physics Communications, 2013, 184, 1861-1873.	3.0	362
8	NOMAD: The FAIR concept for big data-driven materials science. MRS Bulletin, 2018, 43, 676-682.	1.7	288
9	Reconstruction of Molecular Orbital Densities from Photoemission Data. Science, 2009, 326, 702-706.	6.0	282
10	Confined Pyrolysis within Metalâ€“Organic Frameworks To Form Uniform Ru₃ Clusters for Efficient Oxidation of Alcohols. Journal of the American Chemical Society, 2017, 139, 9795-9798.	6.6	258
11	Van der Waals Interactions Between Organic Adsorbates and at Organic/Inorganic Interfaces. MRS Bulletin, 2010, 35, 435-442.	1.7	257
12	Charge distribution and electric-field gradients inYBa2Cu3O7â^'x. Physical Review B, 1990, 42, 2051-2061.	1.1	248
13	exciting: a full-potential all-electron package implementing density-functional theory and many-body perturbation theory. Journal of Physics Condensed Matter, 2014, 26, 363202.	0.7	241
14	First-principles studies of the structural and optical properties of crystalline poly(para-phenylene). Physical Review B, 1995, 51, 9668-9676.	1.1	231
15	Effect of Rhenium on the Dislocation Core Structure in Tungsten. Physical Review Letters, 2010, 104, 195503.	2.9	225
16	Characterization of Step-Edge Barriers in Organic Thin-Film Growth. Science, 2008, 321, 108-111.	6.0	190
17	Theoretical study of PTCDA adsorbed on the coinage metal surfaces, Ag(111), Au(111) and Cu(111). New Journal of Physics, 2009, 11, 053010.	1.2	182
18	Force calculation and atomic-structure optimization for the full-potential linearized augmented plane-wave code WIEN. Computer Physics Communications, 1996, 94, 31-48.	3.0	177

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19	Intra- and Intermolecular Band Dispersion in an Organic Crystal. Science, 2007, 317, 351-355.	6.0	174
20	Electronic properties of oligoacenes from first principles. Physical Review B, 2005, 72, .	1.1	171
21	The NOMAD laboratory: from data sharing to artificial intelligence. JPhys Materials, 2019, 2, 036001.	1.8	171
22	Importance of Van Der Waals Interaction for Organic Molecule-Metal Junctions: Adsorption of Thiophene on Cu(110) as a Prototype. Physical Review Letters, 2007, 99, 176401.	2.9	159
23	Oligoacene exciton binding energies:â€ƒTheir dependence on molecular size. Physical Review B, 2005, 71, .	1.1	152
24	Second-Harmonic Optical Response from First Principles. Physica Scripta, 2004, T109, 128.	1.2	151
25	Crystal and electronic structures of pentacene thin films from grazing-incidence x-ray diffraction and first-principles calculations. Physical Review B, 2007, 76, .	1.1	147
26	Optical absorption spectra of semiconductors and insulators including electron-hole correlations: Anab initiostudy within the LAPW method. Physical Review B, 2002, 66, .	1.1	128
27	Linear and second-order optical response of III-V monolayer superlattices. Physical Review B, 2003, 67, .	1.1	122
28	The role of polymorphism in organic thin films: oligoacenes investigated from first principles. New Journal of Physics, 2009, 11, 125010.	1.2	112
29	Encapsulation of Conjugated Oligomers in Singleâ€Walled Carbon Nanotubes: Towards Nanohybrids for Photonic Devices. Advanced Materials, 2010, 22, 1635-1639.	11.1	112
30	Transport, optical, and electronic properties of the half-metalCrO2. Physical Review B, 1999, 59, 411-418.	1.1	109
31	Epitaxial Growth of Ï€-Stacked Perfluoropentacene on Graphene-Coated Quartz. ACS Nano, 2012, 6, 10874-10883.	7.3	108
32	Influence of the Core-Valence Interaction and of the Pseudopotential Approximation on the Electron Self-Energy in Semiconductors. Physical Review Letters, 2008, 101, 106404.	2.9	107
33	Dislocation-core symmetry and slip planes in tungsten alloys: Ab initio calculations and microcantilever bending experiments. Acta Materialia, 2012, 60, 748-758.	3.8	106
34	Roadmap on organicâ€“inorganic hybrid perovskite semiconductors and devices. APL Materials, 2021, 9, .	2.2	102
35	First-principles calculation of hot-electron scattering in metals. Physical Review B, 2004, 70, .	1.1	101
36	The Dielectric Constant of Selfâ€Assembled Monolayers. Advanced Functional Materials, 2008, 18, 3999-4006.	7.8	101

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37	Optical response of high temperature superconductors by full potential LAPW band structure calculations. Physica B: Condensed Matter, 1994, 194-196, 1451-1452.	1.3	100
38	Orbital tomography: Deconvoluting photoemission spectra of organic molecules. Physical Review B, 2011, 84, .	1.1	99
39	Electronic structure and ferroelectricity inSrBi2Ta2O9. Physical Review B, 2000, 61, 14434-14439.	1.1	95
40	Density-functional study for the oligomers of poly(para-phenylene): Band structures and dielectric tensors. Physical Review B, 1999, 60, 7891-7898.	1.1	94
41	Cohesive and surface energies of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Ï€</mml:mi></mml:math>-conjugated organic molecular crystals: A first-principles study. Physical Review B, 2008, 77, .	1.1	89
42	Lowest Optical Excitations in Molecular Crystals: Bound Excitons versus Free Electron-Hole Pairs in Anthracene. Physical Review Letters, 2004, 92, 147402.	2.9	86
43	Optical absorbance of oriented thin films. Synthetic Metals, 1996, 76, 177-179.	2.1	84
44	FAIR data enabling new horizons for materials research. Nature, 2022, 604, 635-642.	13.7	81
45	Structure, morphology, and optical properties of highly ordered films ofpara-sexiphenyl. Physical Review B, 2000, 61, 16538-16549.	1.1	77
46	Accurate all-electron<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mml:msub></mml:mrow></mml:math> energies employing the full-potential augmented plane-wave method. Physical Review B, 2016, 94, .	1.1	77
47	Organic/Inorganic Hybrid Materials: Challenges for ab Initio Methodology. Accounts of Chemical Research, 2014, 47, 3225-3232.	7.6	75
48	First-Principles Approach to Noncollinear Magnetism: Towards Spin Dynamics. Physical Review Letters, 2007, 98, 196405.	2.9	74
49	Suppression of Electron-Hole Correlations in 3D Polymer Materials. Physical Review Letters, 2002, 89, 056405.	2.9	72
50	All-Electron Exact Exchange Treatment of Semiconductors: Effect of Core-Valence Interaction on Band-Gap andd-Band Position. Physical Review Letters, 2005, 95, 136402.	2.9	70
51	Electronic structure and electric-field gradients forYBa2Cu4O8from density-functional calculations. Physical Review B, 1991, 44, 5141-5147.	1.1	68
52	Time-dependent density functional theory versus Betheâ€“Salpeter equation: an all-electron study. Physical Chemistry Chemical Physics, 2009, 11, 4451.	1.3	67
53	Computing Equilibrium Shapes of Wurtzite Crystals: The Example of GaN. Physical Review Letters, 2015, 115, 085503.	2.9	66
54	Betheâ€“Salpeter equation for absorption and scattering spectroscopy: implementation in the exciting code. Electronic Structure, 2019, 1, 037001.	1.0	66

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55	Ab initiostudy of anthracene under high pressure. Physical Review B, 2003, 67, .	1.1	65
56	All-electron Bethe-Salpeter calculations for shallow-core x-ray absorption near-edge structures. Physical Review B, 2009, 79, .	1.1	65
57	Initial stages of apara-hexaphenyl film growth on amorphous mica. Physical Review B, 2011, 83, .	1.1	65
58	Electronic band structure of pentacene: An experimental and theoretical study. Physical Review B, 2008, 77, .	1.1	63
59	Epitaxy of Rodlike Organic Molecules on Sheet Silicatesâ€”A Growth Model Based on Experiments and Simulations. Journal of the American Chemical Society, 2011, 133, 3056-3062.	6.6	61
60	Optical properties and band structure of2Hâ^'WSe2. Physical Review B, 1999, 60, 8610-8615.	1.1	57
61	Fermi-surface-induced lattice distortion inNbTe2. Physical Review B, 2005, 72, .	1.1	56
62	FHI-gap: A code based on the all-electron augmented plane wave method. Computer Physics Communications, 2013, 184, 348-366.	3.0	56
63	Estimating Excitonic Effects in the Absorption Spectra of Solids: Problems and Insight from a Guided Iteration Scheme. Physical Review Letters, 2015, 114, 146402.	2.9	56
64	Ab initiocalculations of excitons in GaN. Physical Review B, 2005, 72, .	1.1	55
65	Pressure studies on the intermolecular interactions in biphenyl. Synthetic Metals, 2001, 116, 327-331.	2.1	53
66	High pressure x-ray study on anthracene. Journal of Chemical Physics, 2003, 119, 1078-1084.	1.2	52
67	Relativistic effects on the linear optical properties of Au, Pt, Pb and W. New Journal of Physics, 2010, 12, 103048.	1.2	52
68	Interchain interaction and Davydov splitting in polythiophene crystals: An ab initio approach. Applied Physics Letters, 2002, 80, 4118-4120.	1.5	51
69	Polarized absorbance and Davydov splitting in bulk and thin-film pentacene polymorphs. Physical Chemistry Chemical Physics, 2018, 20, 29724-29736.	1.3	50
70	Electric-Magneto-Optical Kerr Effect in a Hybrid Organicâ€“Inorganic Perovskite. Journal of the American Chemical Society, 2017, 139, 12883-12886.	6.6	49
71	OPTIMADE, an API for exchanging materials data. Scientific Data, 2021, 8, 217.	2.4	49
72	Structure Solution of the 6,13-Pentacenequinone Surface-Induced Polymorph by Combining X-ray Diffraction Reciprocal-Space Mapping and Theoretical Structure Modeling. Crystal Growth and Design, 2011, 11, 600-606.	1.4	44

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73	Wannier interpolation scheme for phonon-induced potentials: Application to bulk<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>MgB</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>W, and the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mn>1</mml:mn><mml:mo>Ã—</mml:mo><mml:mn>1</mml:mn></mml:mrow></mml:mrow></mml:math>Physical Review B, 2008, 78, .	1.1	42
74	Structure optimization ofYBa2Cu3O7and its influence on phonons and Fermi surface. Physical Review B, 1999, 60, 9321-9324.	1.1	41
75	Chain-length-dependent intermolecular packing in polyphenylenes: a high pressure study. Journal of Physics Condensed Matter, 2003, 15, 3375-3389.	0.7	41
76	Raman scattering inYBa2Cu3O7:A comprehensive theoretical study in comparison with experiments. Physical Review B, 2002, 65, .	1.1	40
77	Electronic structure of1Tâ^'TiS2. Physical Review B, 1999, 59, 14833-14836.	1.1	38
78	Impact of widely used approximations to theG₀W₀method: an all-electron perspective. New Journal of Physics, 2012, 14, 023006.	1.2	38
79	Electronic, optical, and structural properties of oligophenylene molecular crystals under high pressure: Anab initioinvestigation. Physical Review B, 2003, 67, .	1.1	37
80	Electronic Interactions between â€œPeaâ€•and â€œPodâ€• The Case of Oligothiophenes Encapsulated in Carbon Nanotubes. Small, 2011, 7, 1807-1815.	5.2	37
81	The influence of interstitial carbon on the Î³-surface in austenite. Acta Materialia, 2013, 61, 341-349.	3.8	37
82	Optical spectra from molecules to crystals: Insight from many-body perturbation theory. Physical Review B, 2015, 92, .	1.1	37
83	First-principles calculation of superconductivity in hole-doped LiBC:Tc=65K. Physical Review B, 2003, 68, .	1.1	36
84	Geometry-Dependent Electronic Properties of Highly Fluorescent Conjugated Molecules. Physical Review Letters, 2000, 85, 2388-2391.	2.9	35
85	Influence of Polymorphism on the Electronic Structure of Ga₂O₃. Chemistry of Materials, 2020, 32, 8460-8470.	3.2	35
86	Near-edge structures from first principles all-electron Betheâ€“Salpeter equation calculations. Journal of Physics Condensed Matter, 2009, 21, 104205.	0.7	34
87	Stacking-fault energy and anti-Invar effect in Fe-Mn alloy from first principles. Physical Review B, 2012, 86, .	1.1	33
88	Band renormalization of a polymer physisorbed on graphene investigated by many-body perturbation theory. Physical Review B, 2012, 86, .	1.1	33
89	Photoisomerization for a molecular switch in contact with a surface. Physical Review B, 2012, 85, .	1.1	32
90	State-of-Matter-Dependent Charge-Transfer Interactions between Planar Molecules for Doping Applications. Chemistry of Materials, 2019, 31, 1237-1249.	3.2	32

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91	Electric-field gradient calculations for YBa2Cu3O7-x. Journal of Physics Condensed Matter, 1989, 1, 4491-4496.	0.7	31
92	Dynamic structure factors of Cu, Ag, and Au: Comparative study from first principles. Physical Review B, 2013, 88, .	1.1	31
93	Dimensionality of excitons in stacked van der Waals materials: The example of hexagonal boron nitride. Physical Review B, 2018, 97, .	1.1	31
94	AB-INITIO STUDY ON THE EXCITON BINDING ENERGIES IN ORGANIC SEMICONDUCTORS. Modern Physics Letters B, 2006, 20, 261-280.	1.0	30
95	Magnetic Control of Spin-Orbit Fields: A First-Principles Study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Fe</mml:mi><mml:mo>/</mml:mo><mml:mi>GaAs</mml:mi></mml:math>Junctions. Physical Review Letters, 2013, 111, 036603.	2.9	30
96	Light Controls Polymorphism in Thin Films of Sexithiophene. Crystal Growth and Design, 2015, 15, 1319-1324.	1.4	30
97	Stability and electronic properties of phosphorene oxides: from 0-dimensional to amorphous 2-dimensional structures. Nanoscale, 2017, 9, 2428-2435.	2.8	30
98	Attosecond state-resolved carrier motion in quantum materials probed by soft x-ray XANES. Applied Physics Reviews, 2021, 8, .	5.5	30
99	Hot-electron lifetimes in metals:â€ƒA combinedab initiocalculation and ballistic electron emission spectroscopy analysis. Physical Review B, 2003, 68, .	1.1	29
100	Atomic signatures of local environment from core-level spectroscopy in<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><mml:mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2016, 94, .	1.1	28
101	A momentum space view of the surface chemical bond. Physical Chemistry Chemical Physics, 2011, 13, 3604.	1.3	27
102	Electronic structure ofCrO2as deduced from its magneto-optical Kerr spectra. Physical Review B, 2002, 65, .	1.1	26
103	Phase transition and electronic properties of fluorene: A joint experimental and theoretical high-pressure study. Physical Review B, 2006, 73, .	1.1	26
104	Bound excitons and many-body effects in x-ray absorption spectra of azobenzene-functionalized self-assembled monolayers. Physical Review B, 2015, 92, .	1.1	26
105	Enhanced Lightâ€“Matter Interaction in Graphene/h-BN van der Waals Heterostructures. Journal of Physical Chemistry Letters, 2017, 8, 1464-1471.	2.1	26
106	Band gap renormalization, carrier mobilities, and the electron-phonon self-energy in crystalline naphthalene. Physical Review B, 2020, 101, .	1.1	26
107	Ultrafast Hot Phonon Dynamics in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>MgB</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow> Driven by Anisotropic Electron-Phonon Coupling. Physical Review Letters, 2020, 124, 077001.	2.9	26
108	Accessing the Anisotropic Nonthermal Phonon Populations in Black Phosphorus. Nano Letters, 2021, 21, 6171-6178.	4.5	25

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109	Al<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>L</mml:mi><mml:mrow><mml:mn>2</mml:mn><mml:mo>,</mml:mo><mml:m> x-ray absorption spectra in III-V semiconductors: Many-body perturbation theory in comparison with experiment. Physical Review B, 2011, 83, .	1.1	24
110	Fingerprint of Fractional Charge Transfer at the Metal/Organic Interface. Journal of Physical Chemistry C, 2015, 119, 12538-12544.	1.5	24
111	Predicting Ground-State Configurations and Electronic Properties of the Thermoelectric Clathrates Ba₈Al_xSi_{46â€“x} and Sr₈Al_xSi_{46â€“x}. Chemistry of Materials, 2017, 29, 2414-2424.	3.2	24
112	Fermi-surface topology of rare-earth dihydrides. Physical Review B, 2004, 70, .	1.1	23
113	Self-consistently renormalized quasiparticles under the electron-phonon interaction. Physical Review B, 2009, 79, .	1.1	23
114	Molecular structure of the substrate-induced thin-film phase of tetracene. Journal of Chemical Physics, 2018, 149, 144701.	1.2	23
115	Doping-induced charge redistribution in the high-temperature superconductorHgBa2CuO4+Î´. Physical Review B, 2003, 67, .	1.1	22
116	Complex Quasiparticle Band Structure Induced by Electron-Phonon Interaction: Band Splitting in the1Å—1H/W(110)Surface. Physical Review Letters, 2008, 101, 036402.	2.9	22
117	display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>(100)/Al<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>O<mml:math	1.1	22
118	Exciton-Dominated Core-Level Absorption Spectra of Hybrid Organicâ€“Inorganic Lead Halide Perovskites. Journal of Physical Chemistry Letters, 2018, 9, 1852-1858.	2.1	22
119	Microstructure and Phase Behavior of a Quinquethiophene-Based Self-Assembled Monolayer as a Function of Temperature. Journal of Physical Chemistry C, 2011, 115, 22925-22930.	1.5	21
120	Graphene-modulated photo-absorption in adsorbed azobenzene monolayers. Physical Chemistry Chemical Physics, 2017, 19, 6196-6205.	1.3	21
121	Investigation ofA1gphonons inYBa2Cu3O7by means of linearized-augmented-plane-wave atomic-force calculations. Physical Review B, 1997, 56, 14766-14770.	1.1	20
122	Augmented Planewave Methods. Physica Scripta, 2004, T109, 48.	1.2	20
123	The electronic structure of pentacene revisited. Journal of Electron Spectroscopy and Related Phenomena, 2009, 174, 22-27.	0.8	20
124	Crystal structure determination from two-dimensional powders: A combined experimental and theoretical approach. European Physical Journal: Special Topics, 2009, 167, 59-65.	1.2	20
125	Theoretical analysis of the momentum-dependent loss function of bulk Ag. Ultramicroscopy, 2010, 110, 1081-1086.	0.8	20
126	noloco: An efficient implementation of van der Waals density functionals based on a Monte-Carlo integration technique. Computer Physics Communications, 2011, 182, 1657-1662.	3.0	20

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127	Electronic and optical excitations of two-dimensional <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ZrS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>HfS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml and their heterostructure. Physical Review Materials, 2019, 3, .	0.9	19
128	Lithiation of InSb andCu2Sb:â€ƒA theoretical investigation. Physical Review B, 2004, 70, .	1.1	18
129	Pressure-Induced Hole Doping of the Hg-Based Cuprate Superconductors. Physical Review Letters, 2004, 92, 187004.	2.9	18
130	A full-band -method for solving the Kohnâ€“Sham equation. Computer Physics Communications, 2007, 177, 280-287.	3.0	18
131	Optical properties of azobenzene-functionalized self-assembled monolayers: Intermolecular coupling and many-body interactions. Journal of Chemical Physics, 2016, 145, 234701.	1.2	18
132	Electric field gradient calculations for YBa 2 Cu 3 O 7â^'x. Physica C: Superconductivity and Its Applications, 1989, 162-164, 1353-1354.	0.6	17
133	Excitonic effects in molecular crystals built up by small organic molecules. Chemical Physics, 2006, 325, 3-8.	0.9	17
134	Evidence of Hybrid Excitons in Weakly Interacting Nanopeapods. Journal of Physical Chemistry Letters, 2013, 4, 2664-2667.	2.1	17
135	Energy-Level Alignment at the Interface of Graphene Fluoride and Boron Nitride Monolayers: An Investigation by Many-Body Perturbation Theory. Journal of Physical Chemistry C, 2016, 120, 11671-11678.	1.5	17
136	Resonant electronic Raman scattering in high-Tcsuperconductors. Physical Review B, 2002, 65, .	1.1	16
137	Optical properties, electron-phonon coupling, and Raman scattering of vanadium ladder compounds. Physical Review B, 2004, 70, .	1.1	16
138	Titanium induced polarity inversion in ordered (In,Ga)N/GaN nanocolumns. Nanotechnology, 2016, 27, 065705.	1.3	16
139	First-principles band-structure calculations as a tool for the quantitative interpretation of Raman spectra of high temperature superconductors. Zeitschrift FÂ¼r Physik B-Condensed Matter, 1997, 104, 687-691.	1.1	15
140	Measurement and density functional calculations of optical constants of Ag and Au from infrared to vacuum ultraviolet wavelengths. Physical Review B, 2008, 77, .	1.1	15
141	Combined use of small-angle neutron scattering and atom probe tomography for the analysis of precipitates in a Fe-15 m% Co-25Âm%ÂMo alloy. Applied Physics A: Materials Science and Processing, 2009, 97, 331-340.	1.1	15
142	Energetics and structure of organic molecules embedded in single-wall carbon nanotubes from first principles: The example of benzene. Physical Review B, 2011, 84, .	1.1	15
143	Understanding the effects of packing and chemical terminations on the optical excitations of azobenzene-functionalized self-assembled monolayers. Journal of Physics Condensed Matter, 2017, 29, 394005.	0.7	15
144	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Mo</mml:mi><mml:msub><mml:mi>Te</mml:mi><mml:mi><mml:r as a natural hyperbolic material across the visible and the ultraviolet region. Physical Review Materials, 2020, 4, .	0.9	15

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145	Ab-initio study of excitonic effects in conventional and organic semiconductors. Physica Status Solidi (B): Basic Research, 2005, 242, 1754-1758.	0.7	14
146	First-principles calculation of X-ray dichroic spectra within the full-potential linearized augmented planewave method: An implementation into the Wien2k code. Computer Physics Communications, 2012, 183, 628-636.	3.0	14
147	Diffusive and massive phase transformations in Tiâ€“Alâ€“Nb alloys â€“ Modelling and experiments. Intermetallics, 2013, 38, 126-138.	1.8	14
148	Mapping Atomic Orbitals with the Transmission Electron Microscope: Images of Defective Graphene Predicted from First-Principles Theory. Physical Review Letters, 2016, 117, 036801.	2.9	14
149	Vibrational Effects in X-ray Absorption Spectra of Two-Dimensional Layered Materials. Journal of Physical Chemistry C, 2019, 123, 9688-9692.	1.5	14
150	Optical and electronic properties of crystalline poly(para-phenylene) by first-principles calculations and experimental results. Synthetic Metals, 1995, 69, 411-414.	2.1	13
151	High pressure Raman studies on the structural conformation of oligophenyls. Synthetic Metals, 2001, 116, 163-166.	2.1	13
152	Stress and pressure within the linearized-augmented plane-wave method. Solid State Communications, 2002, 124, 275-282.	0.9	13
153	First-principles study ofHgBa2Canâ^'1CunO2n+2under pressure. Physical Review B, 2004, 69, .	1.1	13
154	Structure optimization effects on the electronic and vibrational properties ofBi2Sr2CaCu2O8. Physical Review B, 2004, 69, .	1.1	13
155	The Be K-edge in beryllium oxide and chalcogenides: soft x-ray absorption spectra from first-principles theory and experiment. Journal of Physics Condensed Matter, 2013, 25, 315501.	0.7	13
156	Electronic and Optical Excitations at the Pyridine/ZnO(101Â¯0) Hybrid Interface. Advanced Theory and Simulations, 2019, 2, 1800108.	1.3	13
157	Multiband electron-phonon coupling in the cuprates: Raman scattering and charge fluctuations. Physical Review B, 2000, 62, 9713-9720.	1.1	12
158	Ab-initio study on the inter-molecular interactions in polythiophene. Synthetic Metals, 2001, 119, 245-246.	2.1	12
159	Electronic properties and Raman spectra of rare-earth carbide halides investigated from first principles. Physical Review B, 2001, 64, .	1.1	12
160	Raman- and infrared-active phonons in superconducting and nonsuperconducting rare-earth transition-metal borocarbides from full-potential calculations. Physical Review B, 2003, 67, .	1.1	12
161	Spin polarization and relativistic electronic structure of the 1Ã—1 H/W(110) surface. New Journal of Physics, 2009, 11, 013056.	1.2	12
162	LayerOptics: Microscopic modeling of optical coefficients in layered materials. Computer Physics Communications, 2016, 201, 119-125.	3.0	12

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