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	Tunability of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>Ga</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math> mathvariant="normal">O</mml:mi></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:math> : Addressing the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î²</mml:mi></mml:math> to <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi></mml:math> phase transition	0.9	4
2	A consistent picture of excitations in cubic BaSnO3 revealed by combining theory and experiment. Communications Materials, 2022, 3, .	2.9	10
3	Electronic Structure of (Organicâ€)Inorganic Metal Halide Perovskites: The Dilemma of Choosing the Right Functional. Advanced Theory and Simulations, 2022, 5, .	1.3	9
4	Numerical quality control for DFT-based materials databases. Npj Computational Materials, 2022, 8, .	3.5	6
5	Rashba and Dresselhaus effects in two-dimensional Pb-I-based perovskites. Physical Review B, 2022, 105, .	1.1	7
6	FAIR data enabling new horizons for materials research. Nature, 2022, 604, 635-642.	13.7	81
7	Hybrid excitations at the interface between a <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> monolayer and organic molecules: A first-principles study. Physical Review Materials, 2022, 6, .	3.1	6
8	Ehrenfest dynamics implemented in the all-electron package exciting. Electronic Structure, 2022, 4, 037001.	1.0	2
9	Attosecond state-resolved carrier motion in quantum materials probed by soft x-ray XANES. Applied Physics Reviews, 2021, 8, .	5.5	30
10	Fingerprints of optical absorption in the perovskite LaInO3 : Insight from many-body theory and experiment. Physical Review B, 2021, 103, .	1.1	6
11	Theoretical description of optical and x-ray absorption spectra of MgO including many-body effects. Physical Review B, 2021, 103, .	1.1	8
12	All-electron full-potential implementation of real-time TDDFT in exciting. Electronic Structure, 2021, 3, 037001.	1.0	6
13	Accessing the Anisotropic Nonthermal Phonon Populations in Black Phosphorus. Nano Letters, 2021, 21, 6171-6178.	4.5	25
14	Influence of carbon on energetics, electronic structure, and mechanical properties of TiAl alloys. New Journal of Physics, 2021, 23, 073048.	1.2	2
15	OPTIMADE, an API for exchanging materials data. Scientific Data, 2021, 8, 217.	2.4	49
16	GIMS: Graphical Interface for Materials Simulations. Journal of Open Source Software, 2021, 6, 2767.	2.0	1
17	Roadmap on organicâ€“inorganic hybrid perovskite semiconductors and devices. APL Materials, 2021, 9, .	2.2	102
18	Tuning two-dimensional electron and hole gases at LaInO3/BaSnO3 interfaces by polar distortions, termination, and thickness. Npj Computational Materials, 2021, 7, .	3.5	5

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19	Influence of Polymorphism on the Electronic Structure of Ga₂O₃. Chemistry of Materials, 2020, 32, 8460-8470.	3.2	35
20	Spatial Confinement as an Effective Strategy for Improving the Catalytic Selectivity in Acetylene Hydrogenation. ACS Applied Materials & Interfaces, 2020, 12, 39352-39361.	4.0	11
21	First-principles study of Pd-alloyed Cu(111) surface in hydrogen atmosphere at realistic temperatures. Journal of Applied Physics, 2020, 128, 145302.	1.1	2
22	Maximally localized Wannier functions within the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>(</mml:mo><mml:mi) Tj ETQq0 0 0 rgBT /Overlock 10 Tf method. Physical Review B, 2020, 101, .	1.1	6
23	High performance solution of skew-symmetric eigenvalue problems with applications in solving the Bethe-Salpeter eigenvalue problem. Parallel Computing, 2020, 96, 102639.	1.3	4
24	Band gap renormalization, carrier mobilities, and the electron-phonon self-energy in crystalline naphthalene. Physical Review B, 2020, 101, .	1.1	26
25	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> Driven by Anisotropic Electron-Phonon Coupling. Physical Review Letters, 2020, 124, 077001.	2.9	26
26	Robust mixing in self-consistent linearized augmented planewave calculations. Electronic Structure, 2020, 2, 037001.	1.0	5
27	Structural, electronic, and optical properties of periodic graphene/h-BN van der Waals heterostructures. Physical Review Materials, 2020, 4, .	0.9	12
28	<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:n as a natural hyperbolic material across the visible and the ultraviolet region. Physical Review Materials, 2020, 4, .	0.9	15
29	Betheâ€“Salpeter equation for absorption and scattering spectroscopy: implementation in the exciting code. Electronic Structure, 2019, 1, 037001.	1.0	66
30	Energy-Level Alignment at Organic/Inorganic Interfaces from First Principles: Example of Poly(para-phenylene)/Rock-Salt ZnO(100). Chemistry of Materials, 2019, 31, 7143-7150.	3.2	6
31	State-of-Matter-Dependent Charge-Transfer Interactions between Planar Molecules for Doping Applications. Chemistry of Materials, 2019, 31, 1237-1249.	3.2	32
32	Electronic and Optical Excitations at the Pyridine/ZnO(101Â¯0) Hybrid Interface. Advanced Theory and Simulations, 2019, 2, 1800108.	1.3	13
33	The NOMAD laboratory: from data sharing to artificial intelligence. JPhys Materials, 2019, 2, 036001.	1.8	171
34	Vibrational Effects in X-ray Absorption Spectra of Two-Dimensional Layered Materials. Journal of Physical Chemistry C, 2019, 123, 9688-9692.	1.5	14
35	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></m 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></m and their heterostructure. Physical Review Materials, 2019, 3, .	0.9	19
36	Crystal-Phase Quantum Wires: One-Dimensional Heterostructures with Atomically Flat Interfaces. Nano Letters, 2018, 18, 247-254.	4.5	7

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37	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
38	Polarized absorbance and Davydov splitting in bulk and thin-film pentacene polymorphs. Physical Chemistry Chemical Physics, 2018, 20, 29724-29736.	1.3	50
39	Molecular structure of the substrate-induced thin-film phase of tetracene. Journal of Chemical Physics, 2018, 149, 144701.	1.2	23
40	NOMAD: The FAIR concept for big data-driven materials science. MRS Bulletin, 2018, 43, 676-682.	1.7	288
41	Dimensionality of excitons in stacked van der Waals materials: The example of hexagonal boron nitride. Physical Review B, 2018, 97, .	1.1	31
42	The LDA-1/2 Method Applied to Atoms and Molecules. Journal of Chemical Theory and Computation, 2018, 14, 4678-4686.	2.3	8
43	Stability and electronic properties of phosphorene oxides: from 0-dimensional to amorphous 2-dimensional structures. Nanoscale, 2017, 9, 2428-2435.	2.8	30
44	Graphene-modulated photo-absorption in adsorbed azobenzene monolayers. Physical Chemistry Chemical Physics, 2017, 19, 6196-6205.	1.3	21
45	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
46	Enhanced Lightâ€“Matter Interaction in Graphene/h-BN van der Waals Heterostructures. Journal of Physical Chemistry Letters, 2017, 8, 1464-1471.	2.1	26
47	Electric-Magneto-Optical Kerr Effect in a Hybrid Organicâ€“Inorganic Perovskite. Journal of the American Chemical Society, 2017, 139, 12883-12886.	6.6	49
48	Valence and conduction band edges of selenide and sulfide-based kesteritesâ€”a study by x-ray based spectroscopy andab initiotheory. Semiconductor Science and Technology, 2017, 32, 104010.	1.0	1
49	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
50	The LDA-1/2 method implemented in the excitingÂcode. Computer Physics Communications, 2017, 220, 263-268.	3.0	7
51	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
52	RigamontietÂal.Reply:. Physical Review Letters, 2016, 117, 159702.	2.9	6
53	Optical properties of azobenzene-functionalized self-assembled monolayers: Intermolecular coupling and many-body interactions. Journal of Chemical Physics, 2016, 145, 234701.	1.2	18
54	Polymorphism in Î±-sexithiophene crystals: relative stability and transition path. Physical Chemistry Chemical Physics, 2016, 18, 14603-14609.	1.3	11

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55	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><mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2016, 94, .	1.1	28
56	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
57	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
58	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
59	LayerOptics: Microscopic modeling of optical coefficients in layered materials. Computer Physics Communications, 2016, 201, 119-125.	3.0	12
60	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
61	Titanium induced polarity inversion in ordered (In,Ga)N/GaN nanocolumns. Nanotechnology, 2016, 27, 065705.	1.3	16
62	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
63	Optical spectra from molecules to crystals: Insight from many-body perturbation theory. Physical Review B, 2015, 92, .	1.1	37
64	Computing Equilibrium Shapes of Wurtzite Crystals: The Example of GaN. Physical Review Letters, 2015, 115, 085503.	2.9	66
65	Fingerprint of Fractional Charge Transfer at the Metal/Organic Interface. Journal of Physical Chemistry C, 2015, 119, 12538-12544.	1.5	24
66	Light Controls Polymorphism in Thin Films of Sexithiophene. Crystal Growth and Design, 2015, 15, 1319-1324.	1.4	30
67	Big Data of Materials Science: Critical Role of the Descriptor. Physical Review Letters, 2015, 114, 105503.	2.9	658
68	Coupling of Hubbard fermions with phonons in La2 CuO4: A combined study using density-functional theory and the generalized tight-binding method. Journal of Alloys and Compounds, 2015, 648, 258-264.	2.8	1
69	First-principles study on lattice instabilities and structural phase transitions in Ba doped La2CuO4. Physica C: Superconductivity and Its Applications, 2015, 517, 20-25.	0.6	9
70	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
71	Organic/Inorganic Hybrid Materials: Challenges for ab Initio Methodology. Accounts of Chemical Research, 2014, 47, 3225-3232.	7.6	75
72	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

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73	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
74	Evidence of Hybrid Excitons in Weakly Interacting Nanopeapods. Journal of Physical Chemistry Letters, 2013, 4, 2664-2667.	2.1	17
75	Dynamic structure factors of Cu, Ag, and Au: Comparative study from first principles. Physical Review B, 2013, 88, .	1.1	31
76	ElaStic: A tool for calculating second-order elastic constants from first principles. Computer Physics Communications, 2013, 184, 1861-1873.	3.0	362
77	Diffusive and massive phase transformations in Tiâ€“Alâ€“Nb alloys â€“ Modelling and experiments. Intermetallics, 2013, 38, 126-138.	1.8	14
78	FHI-gap: A code based on the all-electron augmented plane wave method. Computer Physics Communications, 2013, 184, 348-366.	3.0	56
79	The influence of interstitial carbon on the Î³-surface in austenite. Acta Materialia, 2013, 61, 341-349.	3.8	37
80	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
81	Impact of widely used approximations to theG₀W₀method: an all-electron perspective. New Journal of Physics, 2012, 14, 023006.	1.2	38
82	Photoisomerization for a molecular switch in contact with a surface. Physical Review B, 2012, 85, .	1.1	32
83	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>(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 xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /></mml:msub></mml:math>	1.1	22
84	Stacking-fault energy and anti-Invar effect in Fe-Mn alloy from first principles. Physical Review B, 2012, 86, .	1.1	33
85	Predicting the electronic structure of weakly interacting hybrid systems: The example of nanosized peapod structures. Physical Review B, 2012, 86, .	1.1	9
86	Band renormalization of a polymer physisorbed on graphene investigated by many-body perturbation theory. Physical Review B, 2012, 86, .	1.1	33
87	Epitaxial Growth of Ï€-Stacked Perfluoropentacene on Graphene-Coated Quartz. ACS Nano, 2012, 6, 10874-10883.	7.3	108
88	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
89	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
90	A momentum space view of the surface chemical bond. Physical Chemistry Chemical Physics, 2011, 13, 3604.	1.3	27

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91	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
92	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:mn> x-ray absorption spectra in III-V semiconductors: Many-body perturbation theory in comparison with experiment. Physical Review B, 2011, 83, .	1.1	24
93	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
94	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
95	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
96	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
97	Electronic Interactions between â€œPeaâ€•and â€œPodâ€• The Case of Oligothiophenes Encapsulated in Carbon Nanotubes. Small, 2011, 7, 1807-1815.	5.2	37
98	Initial stages of apara-hexaphenyl film growth on amorphous mica. Physical Review B, 2011, 83, .	1.1	65
99	Orbital tomography: Deconvoluting photoemission spectra of organic molecules. Physical Review B, 2011, 84, .	1.1	99
100	Encapsulation of Conjugated Oligomers in Singleâ€Walled Carbon Nanotubes: Towards Nanohybrids for Photonic Devices. Advanced Materials, 2010, 22, 1635-1639.	11.1	112
101	Theoretical analysis of the momentum-dependent loss function of bulk Ag. Ultramicroscopy, 2010, 110, 1081-1086.	0.8	20
102	ATAT@WIEN2k: An interface for cluster expansion based on the linearized augmented planewave method. Computer Physics Communications, 2010, 181, 913-920.	3.0	10
103	Van der Waals Interactions Between Organic Adsorbates and at Organic/Inorganic Interfaces. MRS Bulletin, 2010, 35, 435-442.	1.7	257
104	Effect of Rhenium on the Dislocation Core Structure in Tungsten. Physical Review Letters, 2010, 104, 195503.	2.9	225
105	Energetics and electronic structure of phenyl-disubstituted polyacetylene: A first-principles study. Physical Review B, 2010, 82, .	1.1	3
106	Relativistic effects on the linear optical properties of Au, Pt, Pb and W. New Journal of Physics, 2010, 12, 103048.	1.2	52
107	Self-consistently renormalized quasiparticles under the electron-phonon interaction. Physical Review B, 2009, 79, .	1.1	23
108	Spin polarization and relativistic electronic structure of the 1Ã—1 H/W(110) surface. New Journal of Physics, 2009, 11, 013056.	1.2	12

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109	Lattice vibrations in CaV₂O₅and their manifestations: a theoretical study based on density functional theory. New Journal of Physics, 2009, 11, 113009.	1.2	3
110	The role of polymorphism in organic thin films: oligoacenes investigated from first principles. New Journal of Physics, 2009, 11, 125010.	1.2	112
111	Angle-resolved photoemission of chain-like molecules: theÂelectronic band structure of sexithiophene and sexiphenyl. Applied Physics A: Materials Science and Processing, 2009, 95, 101-105.	1.1	10
112	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
113	The electronic structure of pentacene revisited. Journal of Electron Spectroscopy and Related Phenomena, 2009, 174, 22-27.	0.8	20
114	Multielectron approach to the electronic structure and mechanisms of superconductivity in high-Tc cuprates. Journal of Magnetism and Magnetic Materials, 2009, 321, 917-919.	1.0	0
115	Excitons in organic semiconductors. Comptes Rendus Physique, 2009, 10, 504-513.	0.3	11
116	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
117	Band-structure topologies of graphene: Spin-orbit coupling effects from first principles. Physical Review B, 2009, 80, .	1.1	579
118	Time-dependent density functional theory versus Betheâ€“Salpeter equation: an all-electron study. Physical Chemistry Chemical Physics, 2009, 11, 4451.	1.3	67
119	All-electron Bethe-Salpeter calculations for shallow-core x-ray absorption near-edge structures. Physical Review B, 2009, 79, .	1.1	65
120	Near-edge structures from first principles all-electron Betheâ€“Salpeter equation calculations. Journal of Physics Condensed Matter, 2009, 21, 104205.	0.7	34
121	Toward an Ab-initio Description of Organic Thin Film Growth. Springer Proceedings in Physics, 2009, , 3-10.	0.1	4
122	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
123	Reconstruction of Molecular Orbital Densities from Photoemission Data. Science, 2009, 326, 702-706.	6.0	282
124	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
125	The role of doping and pressure in Hg based high Tc cuprates: A theoretical study. Current Applied Physics, 2008, 8, 149-152.	1.1	1
126	First-principles approach to the understanding of Ï€-conjugated organic semiconductors. Monatshefte FÃ¼r Chemie, 2008, 139, 389-399.	0.9	6

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127	The Dielectric Constant of Selfâ€Assembled Monolayers. Advanced Functional Materials, 2008, 18, 3999-4006.	7.8	101
128	Characterization of Step-Edge Barriers in Organic Thin-Film Growth. Science, 2008, 321, 108-111.	6.0	190
129	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:ms 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 Physical Review B, 2008, 78, .	1.1	42
130	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
131	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
132	Electronic band structure of pentacene: An experimental and theoretical study. Physical Review B, 2008, 77, .	1.1	63
133	First-principles study of phonons, optical properties, and Raman spectra in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>MgV</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms Physical Review B, 2008, 78, .	1.1	6
134	Complex Quasiparticle Band Structure Induced by Electron-Phonon Interaction: Band Splitting in the1Ã—1H/W(110)Surface. Physical Review Letters, 2008, 101, 036402.	2.9	22
135	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
136	Zone-center phonons inNaV2O5: A comprehensiveab initiostudy including Raman spectra and electron-phonon interaction. Physical Review B, 2007, 75, .	1.1	10
137	First-Principles Approach to Noncollinear Magnetism: Towards Spin Dynamics. Physical Review Letters, 2007, 98, 196405.	2.9	74
138	Intra- and Intermolecular Band Dispersion in an Organic Crystal. Science, 2007, 317, 351-355.	6.0	174
139	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
140	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
141	A full-band -method for solving the Kohnâ€“Sham equation. Computer Physics Communications, 2007, 177, 280-287.	3.0	18
142	Linear optical properties of solids within the full-potential linearized augmented planewave method. Computer Physics Communications, 2006, 175, 1-14.	3.0	1,215
143	Excitonic effects in molecular crystals built up by small organic molecules. Chemical Physics, 2006, 325, 3-8.	0.9	17
144	AB-INITIO STUDY ON THE EXCITON BINDING ENERGIES IN ORGANIC SEMICONDUCTORS. Modern Physics Letters B, 2006, 20, 261-280.	1.0	30

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145	Atomistic Modeling of Optical Properties of Thin Films. Advanced Engineering Materials, 2006, 8, 1151-1155.	1.6	9
146	Linear and nonlinear optical properties of Li under pressure. Physical Review B, 2006, 73, .	1.1	9
147	Inhomogeneity effects in oxygen-dopedHgBa2CuO4. Physical Review B, 2006, 74, .	1.1	7
148	Phase transition and electronic properties of fluorene: A joint experimental and theoretical high-pressure study. Physical Review B, 2006, 73, .	1.1	26
149	Ab-initio study of excitonic effects in conventional and organic semiconductors. Physica Status Solidi (B): Basic Research, 2005, 242, 1754-1758.	0.7	14
150	Influence of pressure on the structure and electronic properties of the layered superconductor Y2C2I2. Journal of Physics Condensed Matter, 2005, 17, S3121-S3130.	0.7	7
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