Friedhelm Bechstedt

List of Publications by Year
in descending order

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597	29,805	4120 87	8599 146
papers	citations	h-index	g-index

606	606	606	19734
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Optical properties of Xenes. , 2022, , 319-352.		0
2	Efficient strain-induced light emission in lonsdaleite germanium. Physical Review Materials, 2021, 5, .	0.9	16
3	Optical Signatures of Dirac Electrodynamics for hBN-Passivated Silicene on Au(111). Nano Letters, 2021, 21, 5301-5307.	4.5	9
4	Beyond graphene: Clean, hydrogenated and halogenated silicene, germanene, stanene, and plumbene. Progress in Surface Science, 2021, 96, 100615.	3.8	42
5	DFT-1/2 method applied to 2D topological insulators: fluorinated and hydrogenated group-IV honeycomb systems. Journal of Physics Condensed Matter, 2021, 33, 435501.	0.7	3
6	Thermal properties of Dirac fermions in Xenes: Model studies. Physical Review B, 2021, 104, .	1.1	1
7	From pseudo-direct hexagonal germanium to direct silicon-germanium alloys. Physical Review Materials, 2021, 5, .	0.9	7
8	Influence of anisotropy, tilt and pairing of Weyl nodes: the Weyl semimetals TaAs, TaP, NbAs and NbP. European Physical Journal B, 2020, 93, 1.	0.6	8
9	Electronic and Optical Properties of Small Metal Fluoride Clusters. ACS Omega, 2020, 5, 13268-13277.	1.6	8
10	Giant excitonic absorption and emission in two-dimensional group-III nitrides. Scientific Reports, 2020, 10, 10719.	1.6	20
11	Direct-bandgap emission from hexagonal Ge and SiGe alloys. Nature, 2020, 580, 205-209.	13.7	231
12	Towards a Hexagonal SiGe Semiconductor Laser.. , 2020, , .		0
13	Transition Matrix Element and Recombination Mechanism of Hexagonal SiGe.. , 2020, , .		0
14	Forbidden Bandâ€Edge Excitons of Wurtziteâ€GaP: A Theoretical View. Physica Status Solidi (B): Basic Research, 2019, 256, 1800238.	0.7	15
15	Charge qubit in van der Waals heterostructures. Physical Review B, 2019, 100, .	1.1	15
16	Out-of-plane excitons in two-dimensional crystals. Physical Review B, 2019, 99, .	1.1	30
17	Influence of screening dynamics on excitons in Ga2O3 polymorphs. Applied Physics Letters, 2019, 114, .	1.5	20
18	Organic Molecule Adsorption on Stepped Siâ€“Au Surfaces: Role of Functional Group on Geometry and Electronic Structure. Physica Status Solidi (B): Basic Research, 2019, 256, 1800653.	0.7	1

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19	Quantization of spin Hall conductivity in two-dimensional topological insulators versus symmetry and spin-orbit interaction. Physical Review B, 2019, 100, .	1.1	25
20	Honeycomb silicon on alumina: Massless Dirac fermions in silicene on substrate. Physical Review B, 2019, 100, .	1.1	17
21	Accurate electronic and optical properties of hexagonal germanium for optoelectronic applications. Physical Review Materials, 2019, 3, .	0.9	41
22	Lattice vibrations and electronic properties of GaSe nanosheets from first principles. Physical Review Materials, 2019, 3, .	0.9	5
23	Trends on band alignments: Validity of Anderson's rule in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SnS</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>SnSe</mml:mi><mml:mn>2</mml:mn></mml:msub></ van der Waals heterostructures. Physical Review B, 2018, 97, .	1.1	57
24	Selective adsorption of toluene-3,4-dithiol on Si(553)-Au surfaces. Physical Review B, 2018, 97, .	1.1	8
25	Efficient Green Emission from Wurtzite Al_xIn_{1â€“x}P Nanowires. Nano Letters, 2018, 18, 3543-3549.	4.5	16
26	Validity of Weyl fermion picture for transition metals monopnictides TaAs, TaP, NbAs, and NbP from ab initio studies. Scientific Reports, 2018, 8, 3534.	1.6	41
27	Optical Properties of Silicene and Related Materials from First Principles. Nanoscience and Technology, 2018, , 73-98.	1.5	6
28	Strong in- and out-of-plane excitons in two-dimensional InN nanosheets. Physical Review B, 2018, 98, .	1.1	26
29	Ab initio optical and energy loss spectra of transition metal monopnictides TaAs, TaP, NbAs, and NbP. Journal of Applied Physics, 2018, 124, .	1.1	6
30	Vibrational properties of GaSe: a layer dependent study from experiments to theory. Semiconductor Science and Technology, 2018, 33, 125008.	1.0	17
31	Spontaneous symmetry breaking and electronic and dielectric properties in commensurate La7/4Sr1/4CuO4 and La5/3Sr1/3NiO4. Physical Review B, 2018, 97, .	1.1	4
32	Electronic excitations stabilized by a degenerate electron gas in semiconductors. Communications Physics, 2018, 1, .	2.0	6
33	Optical properties of silicene, Si/Ag(111), and Si/Ag(110). Physical Review B, 2018, 97, .	1.1	33
34	Correlation beyond the random phase approximation: A consistent many-body perturbation theory approach. Physical Review B, 2018, 97, .	1.1	4
35	Tunable electronic properties of two-dimensional nitrides for light harvesting heterostructures. Applied Physics Letters, 2017, 110, .	1.5	59
36	Tuning Electronic Properties and Band Alignments of Phosphorene Combined With MoSe₂ and WSe₂. Journal of Physical Chemistry C, 2017, 121, 3862-3869.	1.5	55

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37	Fast and accurate approximate quasiparticle band structure calculations of ZnO, CdO, and MgO polymorphs. Physical Review B, 2017, 95, .	1.1	23
38	Electronic and optical properties of topological semimetal Cd3As2. Scientific Reports, 2017, 7, 45500.	1.6	39
39	Optical absorbance and band-gap engineering of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow><mml:mo>(</mml:mo><mml:mi>BN</mml:mi> alloys: Phase s. Physical Review B, 2017, 95, .	1.1	24
40	Deposition of topological silicene, germanene and stanene on graphene-covered SiC substrates. Scientific Reports, 2017, 7, 15700.	1.6	36
41	Chemically Tunable Properties of Graphene Covered Simultaneously with Hydroxyl and Epoxy Groups. Journal of Physical Chemistry C, 2017, 121, 27603-27611.	1.5	6
42	Critical Temperature for the Conversion from Wurtzite to Zincblende of the Optical Emission of InAs Nanowires. Journal of Physical Chemistry C, 2017, 121, 16650-16656.	1.5	2
43	Thermodynamic, electronic, and optical properties of graphene oxide: A statisticalab initioapproach. Physical Review B, 2017, 95, .	1.1	16
44	Coincidence Lattices and Interlayer Twist in van der Waals Heterostructures: Application of the Coincidence Lattice Method on $$hbox {hBN/MoSe}_2$$ hBN/MoSe 2 Heterobilayer Systems. Journal of Electronic Materials, 2017, 46, 3910-3916.	1.0	9
45	Halfâ€Heusler compounds with a 1â€‰eV (1.7â€‰eV) direct band gap, latticeâ€matched to GaAs (Si), for solar cell application: A firstâ€principles study. Physica Status Solidi (B): Basic Research, 2016, 253, 889-894.	0.7	16
46	Pseudodirect to Direct Compositional Crossover in Wurtzite GaP/In_xGa_{1â€“x}P Coreâ€“Shell Nanowires. Nano Letters, 2016, 16, 7930-7936.	4.5	19
47	Optical study of the band structure of wurtzite GaP nanowires. Journal of Applied Physics, 2016, 120, .	1.1	34
48	Hundâ€™s Rule-Driven Dzyaloshinskii-Moriya Interaction at<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi><mml:mtext>â^’</mml:mtext><mml:mn>5</mml:mn><mml: Physical Review Letters, 2016, 117, 247202.	2.9	163
49	Quantum spin Hall phase in stanene-derived overlayers on passivated SiC substrates. Physical Review B, 2016, 94, .	1.1	18
50	Coverage-dependent geometries of nanowires on Ge(0 0 1)-Au surfaces: modification of trenches. Journal of Physics Condensed Matter, 2016, 28, 284005.	0.7	3
51	Influence of the composition fluctuations and decomposition on the tunable direct gap and oscillator strength of Ge1-xSnx alloys. Applied Physics Letters, 2016, 108, 092101.	1.5	19
52	Flexible 2D Crystals of Polycyclic Aromatics Stabilized by Static Distortion Waves. ACS Nano, 2016, 10, 6474-6483.	7.3	23
53	Coincidence Lattices of 2D Crystals: Heterostructure Predictions and Applications. Journal of Physical Chemistry C, 2016, 120, 10895-10908.	1.5	68
54	Optical Properties of Strained Wurtzite Gallium Phosphide Nanowires. Nano Letters, 2016, 16, 3703-3709.	4.5	40

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55	Dipole analysis of the dielectric function of color dispersive materials: Application to monoclinic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ga</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2016, 94, .	1.1	54
56	Ferroelectric phase transitions in multiferroicGe1â^'xMnxTedriven by local lattice distortions. Physical Review B, 2016, 94, .	1.1	13
57	Intrinsic spin Hall conductivity in one-, two-, and three-dimensional trivial and topological systems. Physical Review B, 2016, 94, .	1.1	24
58	Quantum spin Hall effect in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi><mml:mo>â^'</mml:mo><mml:mi mathvariant="normal">Sn</mml:mi><mml:mo>/</mml:mo><mml:mtext>CdTe</mml:mtext><mml:mo>(</mml:mo><mml:mn>001</mml:mn> structures. Physical Review B, 2016, 93, .	1.1	8
59	Quasiparticle bands and spectra of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ga</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>polymorphs. Physical Review B, 2016, 93, .	1.1	165
60	Atomic configurations of Au-induced nanowires on Ge(001) stabilized by higher Au coverages. Physical Review B, 2016, 93, .	1.1	8
61	Quantization and topological states in the spin Hall conductivity of low-dimensional systems: Anab initiostudy. Physical Review B, 2016, 93, .	1.1	12
62	Influence of out-of-plane response on optical properties of two-dimensional materials: First principles approach. Physical Review B, 2016, 94, .	1.1	80
63	Wurtzite silicon as a potential absorber in photovoltaics: Tailoring the optical absorption by applying strain. Physical Review B, 2015, 92, .	1.1	54
64	Influence of structure and thermodynamic stability on electronic properties of two-dimensional SiC, SiGe, and GeC alloys. Physical Review B, 2015, 92, .	1.1	53
65	Spin-dependent properties and images of MnO, FeO, CoO, and NiO(001) surfaces. Physical Review B, 2015, 92, .	1.1	16
66	Near valence-band electronic properties of semiconducting<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î²</mml:mi><mml:msub><mml:mrow><mml:mo>â^'</mml:mo> <mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>(100) single crystals. Physical Review B, 2015, 92, .	1.1	47
67	Dielectric tensor of monoclinic Ga₂O₃ single crystals in the spectral range 0.5â€“8.5 eV. APL Materials, 2015, 3, 106106.	2.2	81
68	Metallic Properties of the Si(111) â^' 5 Ã— 2 â^' Au Surface from Infrared Plasmon Polaritons and Ab Initio Theory. Nano Letters, 2015, 15, 4155-4160.	4.5	27
69	Amorphous Ge quantum dots embedded in crystalline Si:ab initioresults. Journal of Physics Condensed Matter, 2015, 27, 405302.	0.7	12
70	Hamiltonian of Interacting Electrons. Springer Series in Solid-state Sciences, 2015, , 13-27.	0.3	0
71	Topological states in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi><mml:mo>â^'</mml:mo><mml:mi>Sn</mml:mi><mml:mi> HgTe quantum wells: A comparison ofab initioresults. Physical Review B, 2015, 91, .	1.1	20
72	Stability and electronic structure of two-dimensional allotropes of group-IV materials. Physical Review B, 2015, 92, .	1.1	124

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73	Model GW Studies. Springer Series in Solid-state Sciences, 2015, , 327-350.	0.3	0
74	Energies and Forces. Springer Series in Solid-state Sciences, 2015, , 129-161.	0.3	0
75	Metal-to-Insulator Transition in Au Chains on Si(111)-5Ã—2-Au by Band Filling: Infrared Plasmonic Signal and Ab Initio Band Structure Calculation. Journal of Physical Chemistry Letters, 2015, 6, 3615-3620.	2.1	13
76	Many-Body Approach to Electronic Excitations. Springer Series in Solid-state Sciences, 2015, , .	0.3	114
77	Excitons in two-dimensional sheets with honeycomb symmetry. Physica Status Solidi (B): Basic Research, 2015, 252, 72-77.	0.7	23
78	Density Correlation and Electronic Polarization. Springer Series in Solid-state Sciences, 2015, , 255-286.	0.3	0
79	Kohn-Sham Scheme. Springer Series in Solid-state Sciences, 2015, , 89-104.	0.3	0
80	Beyond Static Screening. Springer Series in Solid-state Sciences, 2015, , 539-572.	0.3	0
81	Non-local Exchange and Correlation. Springer Series in Solid-state Sciences, 2015, , 163-195.	0.3	0
82	Silicene on metal and metallized surfaces:ab initiostudies. New Journal of Physics, 2014, 16, 075004.	1.2	24
83	Magnetic exchange force microscopy from first principles: application to the antiferromagnetic NiO(001) surface. New Journal of Physics, 2014, 16, 023020.	1.2	13
84	Modeling of structure and properties of silicene and related novel 2D crystals. , 2014, , .		0
85	Properties of the In2O3-Si interface: An ab initio study of a model geometry. , 2014, , .		0
86	Influence of edge and field effects on topological states of germanene nanoribbons from self-consistent calculations. Physical Review B, 2014, 90, .	1.1	56
87	Topological transition and edge states in HgTe quantum wells from first principles. Physical Review B, 2014, 89, .	1.1	17
88	First-principles calculations of energetics and electronic structure for reconstructed<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Si</mml:mi><mml:mo>(</mml:mo><mml:mn>111</mml:mn><mml:mo>)</mml:mo><mml:mn>2</mml:mn><mml:mo>×</mml:mo><mml:mn>1</mml:mn></mml:mrow></mml:math>Physical Review B, 2014, 90, .	1.1	8
89	Si(111)2Ã—1 surface isomers: DFT investigations on stability and doping effects. Surface Science, 2014, 621, 123-127.	0.8	6
90	Silicene-derived phases on Ag(111) substrate versus coverage:Ab initiostudies. Physical Review B, 2014, 89, .	1.1	60

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91	Unexpected symmetry and AA stacking of bilayer silicene on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Ag</mml:mi><mml:mrow><mml:mn>(111)</mml:mn></mml:mrow></mml:math> Physical Review B, 2014, 89, .	1.1	82
92	Topological<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi></mml:math>-Sn surface states versus film thickness and strain. Physical Review B, 2014, 90, .	1.1	26
93	Optical properties of two-dimensional honeycomb crystals graphene, silicene, germanene, and tinene from first principles. New Journal of Physics, 2014, 16, 105007.	1.2	181
94	One- and two-particle effects in the electronic and optical spectra of barium fluoride. Journal of Physics Condensed Matter, 2014, 26, 125501.	0.7	6
95	Polytypism in ZnS, ZnSe, and ZnTe: First-principles study. Physical Review B, 2014, 89, .	1.1	42
96	Nonmetallic substrates for growth of silicene: anab initioprediction. Journal of Physics Condensed Matter, 2014, 26, 185002.	0.7	45
97	Structural and Magnetic Properties of MnTe Phases from Ab Initio Calculations. Journal of Superconductivity and Novel Magnetism, 2013, 26, 1963-1972.	0.8	26
98	Silicene on hydrogenâ€passivated Si(111) and Ge(111) substrates. Physica Status Solidi - Rapid Research Letters, 2013, 7, 538-541.	1.2	29
99	Universal infrared absorbance of two-dimensional honeycomb group-IV crystals. Physical Review B, 2013, 87, .	1.1	157
100	Structure, energetics, and electronic states of IIIâ€“V compound polytypes. Journal of Physics Condensed Matter, 2013, 25, 273201.	0.7	101
101	Effects of strain on the valence band structure and exciton-polariton energies in ZnO. Physical Review B, 2013, 88, .	1.1	42
102	Massive Dirac quasiparticles in the optical absorbance of graphene, silicene, germanene, and tinene. Journal of Physics Condensed Matter, 2013, 25, 395305.	0.7	179
103	Structural and electronic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-tin nanocrystals from first principles. Physical Review B, 2013, 87, .	1.1	29
104	Origin of Dirac-cone-like features in silicon structures on Ag(111) and Ag(110). Journal of Applied Physics, 2013, 114, .	1.1	68
105	Relation between spontaneous polarization and crystal field from first principles. Physical Review B, 2013, 87, .	1.1	35
106	Theoretical optical spectroscopy of complex systems. Journal of Electron Spectroscopy and Related Phenomena, 2013, 189, 46-55.	0.8	7
107	Enhanced Optical Absorption Due to Symmetry Breaking in TiO_{2(1â€“x)}S_{2x} Alloys. Journal of Physical Chemistry C, 2013, 117, 4189-4193.	1.5	13
108	Electronic and optical properties of cadmium fluoride: The role of many-body effects. Physical Review B, 2013, 87, .	1.1	20

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109	Ab initiocalculation of optical properties with excitonic effects in wurtzite InxGa1â^'xN and InxAl1â^'xN alloys. Physical Review B, 2013, 87, .	1.1	14
110	Direct Band Gap Wurtzite Gallium Phosphide Nanowires. Nano Letters, 2013, 13, 1559-1563.	4.5	262
111	Unit cell structure of the wurtzite phase of GaP nanowires: X-ray diffraction studies and density functional theory calculations. Physical Review B, 2013, 88, .	1.1	28
112	Magnetic anisotropy of FeO and CoO: the influence of gradient corrections on exchange and correlation. Journal of Physics Condensed Matter, 2013, 25, 486002.	0.7	6
113	Optical absorption and emission of Î±-Sn nanocrystals from first principles. Nanotechnology, 2013, 24, 405702.	1.3	13
114	Influence of on-site Coulomb interactionUon properties of MnO(001)2 Ã— 1 and NiO(001)2 Ã— 1 surfaces. Journal of Physics Condensed Matter, 2013, 25, 094006.	0.7	11
115	Magnetic exchange forces andd-state filling: Antiferromagnetic MnO(001) and NiO(001) surfaces. Physical Review B, 2013, 88, .	1.1	4
116	In4d and Ga3d levels in In_xX_{1â^'}_xN (Xâ€‰=â€‰Ga, Al) alloys. Applied Physics Letters, 2013, 102, 172105.	1.5	2
117	Ab-initio study of Mg-doped InN(0001) surface. AIP Advances, 2013, 3, .	0.6	3
118	Side-dependent electron escape from graphene- and graphane-like SiC layers. Applied Physics Letters, 2012, 100, .	1.5	39
119	Real-structure effects: Absorption edge of Mg_xZn_{1-x}O, Cd_xZn_{1-x}O, and n-type ZnO from ab-initio calculations. , 2012, , .		6
120	Large bandwidths in synthetic one-dimensional stacks of biological molecules. Physical Review B, 2012, 86, .	1.1	7
121	Energetics and approximate quasiparticle electronic structure of low-index surfaces of SnO<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>. Physical Review B, 2012, 86, .	1.1	31
122	Structural examination of Au/Ge(001) by surface x-ray diffraction and scanning tunneling microscopy. Physical Review B, 2012, 85, .	1.1	15
123	Band discontinuities at Si-TCO interfaces from quasiparticle calculations: Comparison of two alignment approaches. Physical Review B, 2012, 85, .	1.1	62
124	Ab initio description of quasiparticle band structures and optical near-edge absorption of transparent conducting oxides. Journal of Materials Research, 2012, 27, 2180-2189.	1.2	29
125	Ab initioinvestigation of graphene-based one-dimensional superlattices and their interfaces. Physical Review B, 2012, 86, .	1.1	13
126	Direct experimental determination of the spontaneous polarization of GaN. Physical Review B, 2012, 86, .	1.1	94

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127	Geometric, electronic, and optical properties of the Si(111)2Ã—1 surface: Positive and negative buckling. Physical Review B, 2012, 86, .	1.1	15
128	Electronic bands of III-V semiconductor polytypes and their alignment. Physical Review B, 2012, 86, .	1.1	134
129	Influence of separation of Si nanocrystals embedded in a SiO2 matrix on electronic and optical properties. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2012, 177, 1098-1102.	1.7	4
130	Structural, electrical, and optical properties of hydrogen-doped ZnO films. Physical Review B, 2012, 86, .	1.1	43
131	Crystalline and magnetic anisotropy of the 3<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>d</mml:mi></mml:math>-transition metal monoxides MnO, FeO, CoO, and NiO. Physical Review B, 2012, 86, .	1.1	97
132	Optical and energy-loss spectra of the antiferromagnetic transition metal oxides MnO, FeO, CoO, and NiO including quasiparticle and excitonic effects. Physical Review B, 2012, 86, .	1.1	59
133	[illegible] display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>Ga<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>N and In<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>N. Physical	1.1	22
134	Beyond the<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>approximation: Combining correlation channels. Physical Review B, 2012, 85, .	1.1	69
135	First-Principles Optical Spectra for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>F</mml:mi></mml:math>Centers in MgO. Physical Review Letters, 2012, 108, 126404.	2.9	157
136	Clustering of N impurities in ZnO. Applied Physics Letters, 2012, 100, 022107.	1.5	18
137	Infrared absorbance of silicene and germanene. Applied Physics Letters, 2012, 100, .	1.5	144
138	Strong excitons in novel two-dimensional crystals: Silicane and germanane. Europhysics Letters, 2012, 98, 37004.	0.7	112
139	Tunneling of electrons between Si nanocrystals embedded in a SiO<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>matrix. Physical Review B, 2012, 86, .	1.1	29
140	Surface Properties of Transparent Conducting Oxides from First Principles: In₂O₃, SnO₂, and ZnO. E-Journal of Surface Science and Nanotechnology, 2012, 10, 216-220.	0.1	2
141	Defect induced modification of the surface gap and optical properties of C(111)2â€‰Ã—â€‰1 surface. Physica Status Solidi (A) Applications and Materials Science, 2012, 209, 669-674.	0.8	4
142	Cysteine on Gold: An ab-initio Investigation. , 2012, , 105-117.		0
143	Influence of exchange and correlation on structural and electronic properties of AlN, GaN, and InN polytypes. Physical Review B, 2011, 84, .	1.1	97
144	Tin dioxide from first principles: Quasiparticle electronic states and optical properties. Physical Review B, 2011, 83, .	1.1	145

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145	Electronic and optical properties of Mg_xZn_{1â^'x}O and Cd_xZn_{1â^'x}O fromab initiocalculations. New Journal of Physics, 2011, 13, 085012.	1.2	60
146	Cubic inclusions in hexagonal AlN, GaN, and InN: Electronic states. Physical Review B, 2011, 84, .	1.1	50
147	Polytypism of GaAs, InP, InAs, and InSb: Anab initiostudy. Physical Review B, 2011, 84, .	1.1	47
148	Unit Cell Structure of Crystal Polytypes in InAs and InSb Nanowires. Nano Letters, 2011, 11, 1483-1489.	4.5	117
149	Optical Absorption in Degenerately Doped Semiconductors: Mott Transition or Mahan Excitons?. Physical Review Letters, 2011, 107, 236405.	2.9	61
150	Luminescence and absorption in germanium and silicon nanocrystals: The influence of compression, surface reconstruction, optical excitation, and spin-orbit splitting. Physical Review B, 2011, 83, .	1.1	16
151	Charge transport in organic crystals: Theory and modelling. Physica Status Solidi (B): Basic Research, 2011, 248, 511-525.	0.7	134
152	Effective density of states and carrier masses for Si/SiO₂superlattices from first principles. Semiconductor Science and Technology, 2011, 26, 014024.	1.0	9
153	Interplay of excitonic effects and van Hove singularities in optical spectra: CaO and AlN polymorphs. Physical Review B, 2011, 84, .	1.1	46
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