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	Linear optical properties in the projector-augmented wave methodology. Physical Review B, 2006, 73, .	1.1	2,450
2	Absorption and Emission of Hexagonal InN. Evidence of Narrow Fundamental Band Gap. Physica Status Solidi (B): Basic Research, 2002, 229, r1-r3.	0.7	925
3	Semiempirical van der Waals correction to the density functional description of solids and molecular structures. Physical Review B, 2006, 73, .	1.1	707
4	Quasiparticle band structure based on a generalized Kohn-Sham scheme. Physical Review B, 2007, 76, .	1.1	483
5	Properties of strained wurtzite GaN and AlN:Ab initiostudies. Physical Review B, 2002, 66, .	1.1	375
6	Band gap, electronic structure, and surface electron accumulation of cubic and rhombohedral<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>In</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub	1.1	369
	Physical Review B, 2009, 79, .		
7	Absolute surface energies of group-IV semiconductors: Dependence on orientation and reconstruction. Physical Review B, 2002, 65, .	1.1	366
8	First-principles study of ground- and excited-state properties ofMgO,ZnO, andCdOpolymorphs. Physical Review B, 2006, 73, .	1.1	361
9	Attracted by Long-Range Electron Correlation: Adenine on Graphite. Physical Review Letters, 2005, 95, 186101.	2.9	275
10	Band Gap of InN and In-Rich InxGa1?xN alloys (0.36 < x < 1). Physica Status Solidi (B): Basic Research, 2002, 230, R4-R6.	0.7	272
11	Band Gap of Hexagonal InN and InGaN Alloys. Physica Status Solidi (B): Basic Research, 2002, 234, 787-795.	0.7	265
12	Direct Band Gap Wurtzite Gallium Phosphide Nanowires. Nano Letters, 2013, 13, 1559-1563.	4.5	262
13	Optical properties of semiconductors using projector-augmented waves. Physical Review B, 2001, 63, .	1.1	259
14	Quasiparticle band structures of the antiferromagnetic transition-metal oxides MnO, FeO, CoO, and NiO. Physical Review B, 2009, 79, .	1.1	243
15	Direct-bandgap emission from hexagonal Ge and SiGe alloys. Nature, 2020, 580, 205-209.	13.7	231
16	Ab initiolattice dynamics of BN and AlN: Covalent versus ionic forces. Physical Review B, 1997, 56, 7404-7415.	1.1	228
17	Vacancies in SiC: Influence of Jahn-Teller distortions, spin effects, and crystal structure. Physical Review B, 1999, 59, 15166-15180.	1.1	225
18	Polytypism and Properties of Silicon Carbide. Physica Status Solidi (B): Basic Research, 1997, 202, 35-62.	0.7	223

#	Article	IF	Citations
19	Indium-oxide polymorphs from first principles: Quasiparticle electronic states. Physical Review B, 2008, 77, .	1.1	219
20	Origin of electron accumulation at wurtzite InN surfaces. Physical Review B, 2004, 69, .	1.1	205
21	Principles of Surface Physics. Advanced Texts in Physics, 2003, , .	0.5	195
22	First-principles calculations of the thermodynamic and structural properties of strainedInxGa1â^'xNandAlxGa1â^'xNalloys. Physical Review B, 2000, 62, 2475-2485.	1.1	187
23	Phonon deformation potentials of Î±-GaN and -AlN: An ab initio calculation. Applied Physics Letters, 2000, 77, 346-348.	1.5	185
24	Ab initiostudy of structural, dielectric, and dynamical properties of GaN. Physical Review B, 1998, 57, 7043-7049.	1.1	181
25	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
26	Massive Dirac quasiparticles in the optical absorbance of graphene, silicene, germanene, and tinene. Journal of Physics Condensed Matter, 2013, 25, 395305.	0.7	179
27	Branch-point energies and band discontinuities of III-nitrides and III-/II-oxides from quasiparticle band-structure calculations. Applied Physics Letters, 2009, 94, .	1.5	177
28	First-principles calculations of gap bowing inInxGa1â^'xNandInxAl1â^'xNalloys: Relation to structural and thermodynamic properties. Physical Review B, 2002, 65, .	1.1	172
29	Novel Reconstruction Mechanism for Dangling-Bond Minimization: Combined Method Surface Structure Determination ofSiC(111)-(3Â—3). Physical Review Letters, 1998, 80, 758-761.	2.9	170
30	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: 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
31	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
32	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
33	Universal infrared absorbance of two-dimensional honeycomb group-IV crystals. Physical Review B, 2013, 87, .	1.1	157
34	Tin dioxide from first principles: Quasiparticle electronic states and optical properties. Physical Review B, 2011, 83, .	1.1	145
35	Electronic properties of cubic and hexagonal SiC polytypes fromab initiocalculations. Physical Review B, 1994, 50, 10761-10768.	1.1	144
36	Infrared absorbance of silicene and germanene. Applied Physics Letters, 2012, 100, .	1.5	144

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37	Optical and energy-loss spectra of MgO, ZnO, and CdO fromab initiomany-body calculations. Physical Review B, 2009, 80, .	1.1	142
38	Model dielectric function for semiconductors. Physical Review B, 1993, 47, 9892-9895.	1.1	137
39	Nonlocality and many-body effects in the optical properties of semiconductors. Physical Review B, 1996, 53, 9797-9808.	1.1	137
40	An efficient method for calculating quasiparticle energies in semiconductors. Solid State Communications, 1992, 84, 765-770.	0.9	136
41	Influence of atomic relaxations on the structural properties of SiC polytypes fromab initiocalculations. Physical Review B, 1994, 50, 17037-17046.	1.1	136
42	Model GW band structure ofInAsandGaAsin the wurtzite phase. Physical Review B, 2007, 75, .	1.1	136
43	Properties of hexagonal polytypes of group-IV elements from first-principles calculations. Physical Review B, 2002, 66, .	1.1	134
44	EfficientO(N2)method to solve the Bethe-Salpeter equation. Physical Review B, 2003, 67, .	1.1	134
45	Charge transport in organic crystals: Theory and modelling. Physica Status Solidi (B): Basic Research, 2011, 248, 511-525.	0.7	134
46	Electronic bands of III-V semiconductor polytypes and their alignment. Physical Review B, 2012, 86, .	1.1	134
47	Coulombic Amino Group-Metal Bonding: Adsorption of Adenine on Cu(110). Physical Review Letters, 2005, 94, 236102.	2.9	131
48	Theory of charge transport in organic crystals: Beyond Holsteinâ€™s small-polaron model. Physical Review B, 2009, 79, .	1.1	131
49	Analytical treatment of band-gap underestimates in the local-density approximation. Physical Review B, 1988, 38, 7710-7716.	1.1	128
50	Numerical calculation of the optical absorption in semiconductor quantum structures. Physical Review B, 1996, 54, 11592-11601.	1.1	124
51	Valence-band electronic structure of CdO, ZnO, and MgO from x-ray photoemission spectroscopy and quasi-particle-corrected density-functional theory calculations. Physical Review B, 2009, 79, .	1.1	124
52	Stability and electronic structure of two-dimensional allotropes of group-IV materials. Physical Review B, 2015, 92, .	1.1	124
53	Pressure-dependent properties of SiC polytypes. Physical Review B, 1996, 53, 13400-13413.	1.1	123
54	Phonons in ternary group-III nitride alloys. Physical Review B, 2000, 61, 6091-6105.	1.1	123

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55	Optical Absorption of Water: Coulomb Effects versus Hydrogen Bonding. Physical Review Letters, 2005, 94, 037404.	2.9	123
56	Heterocrystalline Structures: New Types of Superlattices?. Physical Review Letters, 1995, 75, 2180-2183.	2.9	122
57	Abâ€initio theory of semiconductor band structures: New developments and progress. Physica Status Solidi (B): Basic Research, 2009, 246, 1877-1892.	0.7	120
58	Bulk Excitonic Effects in Surface Optical Spectra. Physical Review Letters, 2001, 88, 016402.	2.9	117
59	Do we know the fundamental energy gap of InN?. Journal of Crystal Growth, 2002, 246, 315-319.	0.7	117
60	Efficient<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="script">O</mml:mi><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:msup><mml:mi>N</mml:mi><mml:mn>2</mml:m to solve the Bethe-Salpeter equation for excitonic bound states. Physical Review B, 2008, 78, .	1.1	117
61	Unit Cell Structure of Crystal Polytypes in InAs and InSb Nanowires. Nano Letters, 2011, 11, 1483-1489.	4.5	117
62	Pressure dependence of the dielectric and lattice-dynamical properties of GaN and AlN. Physical Review B, 2000, 62, 4526-4534.	1.1	114
63	Shape of free and constrained group-IV crystallites: Influence of surface energies. Physical Review B, 2005, 72, .	1.1	114
64	Many-Body Approach to Electronic Excitations. Springer Series in Solid-state Sciences, 2015, , .	0.3	114
65	Strong excitons in novel two-dimensional crystals: Silicane and germanane. Europhysics Letters, 2012, 98, 37004.	0.7	112
66	High-precision determination of atomic positions in crystals: The case of6H- and4H-SiC. Physical Review B, 1998, 57, 2647-2650.	1.1	110
67	Quasiparticle band structure of silicon carbide polytypes. Physical Review B, 1995, 52, 10897-10905.	1.1	109
68	Free-carrier absorption in nitrides from first principles. Physical Review B, 2010, 81, .	1.1	109
69	Dynamics and polarization of group-III nitride lattices:â€‚A first-principles study. Physical Review B, 2000, 62, 8003-8011.	1.1	108
70	Band structures and optical spectra of InN polymorphs: Influence of quasiparticle and excitonic effects. Physical Review B, 2005, 72, .	1.1	108
71	Reflectance Anisotropy of GaAs(100): Theory and Experiment. Physical Review Letters, 1998, 81, 721-724.	2.9	106
72	Determination of the branch-point energy of InN: Chemical trends in common-cation and common-anion semiconductors. Physical Review B, 2008, 77, .	1.1	106

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73	Extreme softening of Vanderbilt pseudopotentials: General rules and case studies of first-row andd-electron elements. Physical Review B, 2000, 61, 4576-4587.	1.1	102
74	Phase separation suppression in InGaN epitaxial layers due to biaxial strain. Applied Physics Letters, 2002, 80, 769-771.	1.5	102
75	Universality of electron accumulation at wurtzite c- and a-plane and zinc-blende InN surfaces. Applied Physics Letters, 2007, 91, 092101.	1.5	102
76	Alkali adsorption on GaAs(110): atomic structure, electronic states and surface dipoles. Surface Science Reports, 1993, 18, 145-198.	3.8	101
77	Structure, energetics, and electronic states of IIIâ€“V compound polytypes. Journal of Physics Condensed Matter, 2013, 25, 273201.	0.7	101
78	Compensation of Dynamical Quasiparticle and Vertex Corrections in Optical Spectra. Physical Review Letters, 1997, 78, 1528-1531.	2.9	99
79	Adsorption of group-V elements on IIIâ€“V (1 1 0) surfaces. Surface Science Reports, 1996, 25, 141-223.	3.8	97
80	Influence of exchange and correlation on structural and electronic properties of AlN, GaN, and InN polytypes. Physical Review B, 2011, 84, .	1.1	97
81	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
82	Raman Frequencies and Angular Dispersion of Polar Modes in Aluminum Nitride and Gallium Nitride. Physica Status Solidi (B): Basic Research, 1996, 198, 621-627.	0.7	96
83	Raman spectra of isotopic GaN. Physical Review B, 1997, 56, 14399-14406.	1.1	96
84	Optical properties of Ge and Si nanocrystallites fromab initiocalculations. II. Hydrogenated nanocrystallites. Physical Review B, 2002, 65, .	1.1	94
85	Direct experimental determination of the spontaneous polarization of GaN. Physical Review B, 2012, 86, .	1.1	94
86	Lattice dynamics of SiC polytypes within the bond-charge model. Physical Review B, 1994, 50, 13401-13411.	1.1	92
87	Geometry and electronic structure of GaAs(001)(2Ã—4) reconstructions. Physical Review B, 1996, 54, 16742-16748.	1.1	92
88	Energy gap and optical properties of InxGa1xN. Physica Status Solidi A, 2003, 195, 628-633.	1.7	92
89	Ground- and excited-state properties of DNA base molecules from plane-wave calculations using ultrasoft pseudopotentials. Journal of Computational Chemistry, 2004, 25, 112-122.	1.5	88
90	Understanding reflectance anisotropy: Surface-state signatures and bulk-related features in the optical spectrum ofInP(001)(2Ã—4). Physical Review B, 2000, 61, R16335-R16338.	1.1	87

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91	Stacking faults in group-IV crystals: Anab initiostudy. Physical Review B, 1998, 58, 1326-1330.	1.1	85
92	Influence of polytypism on thermal properties of silicon carbide. Physical Review B, 1996, 54, 1791-1798.	1.1	82
93	Optical functions of semiconductors beyond density-functional theory and random-phase approximation. Physical Review B, 1997, 55, 4343-4352.	1.1	81
94	Second-harmonic polarizability including electron-hole attraction from band-structure theory. Physical Review B, 2005, 71, .	1.1	81
95	Dielectric tensor of monoclinic Ga₂O₃ single crystals in the spectral range 0.5â€“8.5 eV. APL Materials, 2015, 3, 106106.	2.2	81
96	Surface phase diagram of (2Ã—4) and (4Ã—2) reconstructions of GaAs(001). Physical Review B, 2000, 62, 8087-8091.	1.1	80
97	MBE growth and properties of SiC multi-quantum well structures. Applied Surface Science, 2001, 184, 37-42.	3.1	80
98	Influence of out-of-plane response on optical properties of two-dimensional materials: First principles approach. Physical Review B, 2016, 94, .	1.1	80
99	Ab initiotheory of excitons and optical properties for spin-polarized systems: Application to antiferromagnetic MnO. Physical Review B, 2008, 77, .	1.1	79
100	Observation of quantized subband states and evidence for surface electron accumulation in CdO from angle-resolved photoemission spectroscopy. Physical Review B, 2008, 78, .	1.1	75
101	Si-richSiC(111)/(0001)3Ã—3and3Ã—3surfaces: A Mott-Hubbard picture. Physical Review B, 1998, 58, 13712-13716	1.1	73
102	Total energy minimization for surfaces of covalent semiconductors C, Si, Ge, and Î±-Sn. Surface Science, 1988, 202, 83-98.	0.8	71
103	Raman studies on phonon modes in cubic AlGaN alloy. Applied Physics Letters, 1999, 74, 191-193.	1.5	71
104	Ab initio calculation of structural, lattice dynamical, and thermal properties of cubic silicon carbide. International Journal of Quantum Chemistry, 1995, 56, 801-817.	1.0	70
105	Band structure of ZnO from resonant x-ray emission spectroscopy. Physical Review B, 2008, 78, .	1.1	70
106	Charge transport in organic crystals: interplay of band transport, hopping and electronâ€“phonon scattering. New Journal of Physics, 2010, 12, 023011.	1.2	70
107	Lattice parameter and energy band gap of cubic AlxGayIn1âˆ’xâˆ’yN quaternary alloys. Applied Physics Letters, 2003, 83, 890-892.	1.5	69
108	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

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109	InP(001)-(2Ã—1) Surface: A Hydrogen Stabilized Structure. Physical Review Letters, 2003, 90, 126101.	2.9	68
110	Bandâ€structure and opticalâ€transition parameters of wurtzite MgO, ZnO, and CdO from quasiparticle calculations. Physica Status Solidi (B): Basic Research, 2009, 246, 2150-2153.	0.7	68
111	Origin of Dirac-cone-like features in silicon structures on Ag(111) and Ag(110). Journal of Applied Physics, 2013, 114, .	1.1	68
112	Coincidence Lattices of 2D Crystals: Heterostructure Predictions and Applications. Journal of Physical Chemistry C, 2016, 120, 10895-10908.	1.5	68
113	Bond-rotation versus bond-contraction relaxation of (110) surfaces of group-III nitrides. Physical Review B, 1998, 58, R1722-R1725.	1.1	67
114	Geometry and electronic structure of InP(001)(2Ã—4) reconstructions. Surface Science, 1998, 409, 474-484.	0.8	66
115	Surface influence on stability and structure of hexagon-shaped III-V semiconductor nanorods. Journal of Applied Physics, 2007, 102, 063528.	1.1	66
116	Long-Range Surface Reconstruction:Si(110)â˜'(16Ã—2). Physical Review Letters, 2004, 93, 136104.	2.9	65
117	Structure- and spin-dependent excitation energies and lifetimes of Si and Ge nanocrystals fromab initiocalculations. Physical Review B, 2004, 69, .	1.1	65
118	Quasiparticle bands and optical spectra of highly ionic crystals: AlN and NaCl. Physical Review B, 2005, 72, .	1.1	65
119	Organic molecule adsorption on solid surfaces: chemical bonding, mutual polarisation and dispersion interaction. Applied Physics A: Materials Science and Processing, 2006, 85, 387-397.	1.1	65
120	Theoretical study of the chemical gap tuning in silicon nanowires. Physical Review B, 2007, 76, .	1.1	65
121	Atomic structure of InP(001)-(2Ã—4): A dimer reconstruction. Physical Review B, 1998, 57, 14596-14599.	1.1	64
122	Origin of the Different Reconstructions of Diamond, Si, and Ge(111) Surfaces. Physical Review Letters, 2001, 87, 016103.	2.9	64
123	Molecular electronic excitations calculated from a solid-state approach: Methodology and numerics. Physical Review B, 2005, 72, .	1.1	64
124	Optical spectra of Si nanocrystallites: Bethe-Salpeter approach versus time-dependent density-functional theory. Physical Review B, 2008, 78, .	1.1	64
125	Spin state of vacancies: From magnetic Jahn-Teller distortions to multiplets. Physical Review B, 2000, 62, 6854-6857.	1.1	63
126	Structure of the diamond (111) surface: Single-dangling-bond versus triple-dangling-bond face. Physical Review B, 1996, 53, 13725-13733.	1.1	62

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127	Energetic stability and magnetic properties of MnO in the rocksalt, wurtzite, and zinc-blende structures: Influence of exchange and correlation. Physical Review B, 2010, 82, .	1.1	62
128	Band discontinuities at Si-TCO interfaces from quasiparticle calculations: Comparison of two alignment approaches. Physical Review B, 2012, 85, .	1.1	62
129	Quasiparticle corrections for energy gaps in semiconductors. , 1992, , 161-177.		61
130	Terrace and step contributions to the optical anisotropy of Si(001) surfaces. Physical Review B, 2001, 63, .	1.1	61
131	Optical Absorption in Degenerately Doped Semiconductors: Mott Transition or Mahan Excitons?. Physical Review Letters, 2011, 107, 236405.	2.9	61
132	Anisotropy of the dielectric function for wurtzite InN. Superlattices and Microstructures, 2004, 36, 591-597.	1.4	60
133	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
134	Silicene-derived phases on Ag(111) substrate versus coverage:Ab initiostudies. Physical Review B, 2014, 89, .	1.1	60
135	III-V(110) surface dynamics from anab initiofrozen-phonon approach. Physical Review B, 1995, 52, 2001-2007.	1.1	59
136	Field-Induced Delocalization and Zener Breakdown in Semiconductor Superlattices. Physical Review Letters, 2001, 86, 1307-1310.	2.9	59
137	Structural relaxation in Si and Ge nanocrystallites: Influence on the electronic and optical properties. Physical Review B, 2003, 67, .	1.1	59
138	Energetics of Si(001) Surfaces Exposed to Electric Fields and Charge Injection. Physical Review Letters, 2004, 93, 036101.	2.9	59
139	Hexagon versus Trimer Formation in In Nanowires on Si(111): Energetics and Quantum Conductance. Physical Review Letters, 2007, 98, 026105.	2.9	59
140	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
141	Tunable electronic properties of two-dimensional nitrides for light harvesting heterostructures. Applied Physics Letters, 2017, 110, .	1.5	59
142	Lattice relaxation around substitutional defects in semiconductors. Physical Review B, 1989, 39, 5041-5050.	1.1	58
143	Geometrical and electronic structure of the reconstructed diamond (100) surface. Physical Review B, 1994, 50, 17697-17700.	1.1	58
144	Influence of SiO₂matrix on electronic and optical properties of Si nanocrystals. Nanotechnology, 2009, 20, 135702.	1.3	58

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145	Optical properties of Ge and Si nanocrystallites fromab initiocalculations. I. Embedded nanocrystallites. Physical Review B, 2002, 65, .	1.1	57
146	Valence-band structure of InN from x-ray photoemission spectroscopy. Physical Review B, 2005, 72, .	1.1	57
147	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
148	Effect of backbond oxidation on silicon nanocrystallites. Physical Review B, 2004, 70, .	1.1	56
149	Influence of edge and field effects on topological states of germanene nanoribbons from self-consistent calculations. Physical Review B, 2014, 90, .	1.1	56
150	Electronic Relaxation Effects in Core Level Spectra of Solids. Physica Status Solidi (B): Basic Research, 1982, 112, 9-49.	0.7	55
151	Validity of effective-medium theory for optical properties of embedded nanocrystallites fromab initiosupercell calculations. Physical Review B, 2003, 67, .	1.1	55
152	Structural elements on reconstructed Si andGe(110)surfaces. Physical Review B, 2004, 70, .	1.1	55
153	Strain influence on valence-band ordering and excitons in ZnO: Anab initiostudy. Applied Physics Letters, 2007, 91, 241915.	1.5	55
154	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
155	GW self-energy calculations for systems with huge supercells. Physical Review B, 2002, 66, .	1.1	54
156	P-richGaP(001)(2Ã—1)/(2Ã—2)surface:â€‚â€‚A hydrogen-adsorbate structure determined from first-principles calculations. Physical Review B, 2003, 68, .	1.1	54
157	Wurtzite silicon as a potential absorber in photovoltaics: Tailoring the optical absorption by applying strain. Physical Review B, 2015, 92, .	1.1	54
158	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
159	GaAs(001): Surface Structure and Optical Properties. Physica Status Solidi A, 2001, 188, 1401-1409.	1.7	53
160	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
161	Dielectric Screening, Polar Phonons, and Longitudinal Electronic Excitations of Quantum Well Double Heterostructures Application to Light Scattering from Charge Density Fluctuations. Physica Status Solidi (B): Basic Research, 1985, 131, 53-66.	0.7	51
162	Structural properties ofPbTeâˆ•CdTeinterfaces from first principles. Physical Review B, 2006, 74, .	1.1	51

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163	Characterization of carbon-carbon bonds on the SiC(001)c(2Ã—2) surface. Physical Review B, 1996, 54, 10304-10307.	1.1	50
164	Cubic inclusions in hexagonal AlN, GaN, and InN: Electronic states. Physical Review B, 2011, 84, .	1.1	50
165	Lattice dynamics of GaN: Effects of3delectrons. Physical Review B, 1997, 56, 3560-3563.	1.1	49
166	Quantum confinement in Si- and Ge-capped nanocrystallites. Physical Review B, 2005, 72, .	1.1	49
167	Ab initiodescription of heterostructural alloys: Thermodynamic and structural properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Mg</mml:mtext></mml:mrow><mml:mi>x</mml:mi></mml:ms xmlns:mml="http://www.w3.org/1998/Math/MathM. Physical Review B, 2010, 81, .	1.1	49
168	Relationship of Microscopic and Macroscopic Theories for Longâ€Wavelength Optical Phonons in GaAsâ€AlAs Superlattices. Physica Status Solidi (B): Basic Research, 1989, 156, 151-170.	0.7	48
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