Walter R L Lambrecht

List of Publications by Year
in descending order

268	13,492	24978	27345
papers	citations	h-index	g-index

281	281	281	11642
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quasiparticle band structure calculation of monolayer, bilayer, and bulk MoS<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, 85, .	1.1	1,127
2	Elastic constants and related properties of tetrahedrally bonded BN, AlN, GaN, and InN. Physical Review B, 1996, 53, 16310-16326.	1.1	670
3	Minimal basis sets in the linear muffin-tin orbital method: Application to the diamond-structure crystals C, Si, and Ge. Physical Review B, 1986, 34, 2439-2449.	1.1	434
4	Electronic band structure, phonons, and exciton binding energies of halide perovskites CsSnCl<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>, CsSnBr<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>, and CsSnI<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mm	1.1	404
5	Efficientab initiomethod for the calculation of frequency-dependent second-order optical response in semiconductors. Physical Review B, 1998, 57, 3905-3919.	1.1	371
6	Electronic structure of rare-earth nitrides using theLSDA+Uapproach: Importance of allowing4forbitals to break the cubic crystal symmetry. Physical Review B, 2007, 75, .	1.1	332
7	Calculated elastic constants and deformation potentials of cubic SiC. Physical Review B, 1991, 44, 3685-3694.	1.1	290
8	Diamond nucleation by hydrogenation of the edges of graphitic precursors. Nature, 1993, 364, 607-610.	13.7	271
9	Valence-band ordering and magneto-optic exciton fine structure in ZnO. Physical Review B, 2002, 65, .	1.1	241
10	Second-harmonic generation of I-III-VI2chalcopyrite semiconductors: Effects of chemical substitutions. Physical Review B, 2001, 63, .	1.1	237
11	Electronic and crystal structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Cu</mml:mi><mml:mrow><mml:mn>2</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">S</mml:mi></mml:mrow></mml:math>: Full-potential electronic structure calculations. Physical Review B, 2007, 76, .	1.1	230
12	Effective masses and valence-band splittings in GaN and AlN. Physical Review B, 1997, 56, 7363-7375.	1.1	226
13	Valenceâ€band discontinuity between GaN and AlN measured by xâ€ray photoemission spectroscopy. Applied Physics Letters, 1994, 65, 610-612.	1.5	212
14	Electronic structure of GaN with strain and phonon distortions. Physical Review B, 1994, 50, 1502-1505.	1.1	198
15	Theoretical study of the relative stability of wurtzite and rocksalt phases in MgO and GaN. Physical Review B, 2001, 63, .	1.1	168
16	Stacking fault band structure in 4Hâ€“SiC and its impact on electronic devices. Applied Physics Letters, 2001, 79, 4360-4362.	1.5	162
17	High field electron transport properties of bulk ZnO. Journal of Applied Physics, 1999, 86, 6864-6867.	1.1	160
18	Electronic structure and optical spectra of the semimetal ScAs and of the indirect-band-gap semiconductors ScN and GdN. Physical Review B, 2000, 62, 13538-13545.	1.1	159

#	Article	IF	Citations
19	Self-consistent dipole theory of heterojunction band offsets. Physical Review B, 1990, 41, 2813-2831.	1.1	148
20	Homogeneous Strain Deformation Path for the Wurtzite to Rocksalt High-Pressure Phase Transition in GaN. Physical Review Letters, 2001, 86, 91-94.	2.9	140
21	First-principles calculation of the O vacancy in ZnO: A self-consistent gap-corrected approach. Physical Review B, 2008, 77, .	1.1	137
22	Quasiparticle band structure of Zn-IV-N<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>compounds. Physical Review B, 2011, 84, .	1.1	134
23	Electronic band structure trends of perovskite halides: Beyond Pb and Sn to Ge and Si. Physical Review B, 2016, 93, .	1.1	130
24	Rare-earth mononitrides. Progress in Materials Science, 2013, 58, 1316-1360.	16.0	124
25	Electronic structure of rare-earth pnictides. Physical Review B, 1996, 53, 4324-4339.	1.1	119
26	Electronic structure and bonding at SiC/AlN and SiC/BP interfaces. Physical Review B, 1991, 43, 7070-7085.	1.1	116
27	Total energy differences between SiC polytypes revisited. Physical Review B, 1998, 57, 12017-12022.	1.1	106
28	Electronic structure and properties ofNiSi2andCoSi2in the fluorite and adamantane structures. Physical Review B, 1987, 36, 2493-2503.	1.1	105
29	Anomalous band-gap behavior and phase stability ofc-BNâ€“diamond alloys. Physical Review B, 1993, 47, 9289-9296.	1.1	105
30	Electronic structure and equilibrium properties ofGaxAl1âˆ’xN alloys. Physical Review B, 1993, 48, 17841-17847.	1.1	103
31	X-ray photoelectron spectroscopy and theory of the valence band and semicore Ga 3dstates in GaN. Physical Review B, 1994, 50, 14155-14160.	1.1	101
32	Atomic-Scale Spin-Polarized Scanning Tunneling Microscopy Applied toMn3N2(010). Physical Review Letters, 2002, 89, 226101.	2.9	100
33	Electronic band structure of ordered vacancy defect chalcopyrite compounds with formulaIIâˆ’III2âˆ’VI4. Physical Review B, 2004, 69, .	1.1	96
34	Charge-neutral disorder and polytypes in heterovalent wurtzite-based ternary semiconductors: The importance of the octet rule. Physical Review B, 2015, 91, .	1.1	95
35	Band offsets between ZnGeN<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>, GaN, ZnO, and ZnSnN<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>and their potential impact for solar cells. Physical Review B, 2013, 88, .	1.1	89
36	Second-harmonic generation and birefringence of some ternary pnictide semiconductors. Physical Review B, 1999, 59, 2737-2748.	1.1	87

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37	Pressure-dependent elastic constants and sound velocities of wurtzite SiC, GaN, InN, ZnO, and CdSe, and their relation to the high-pressure phase transition: A first-principles study. Physical Review B, 2010, 82, .	1.1	87
38	Magnetic properties of substitutional3dtransition metal impurities in silicon carbide. Physical Review B, 2003, 68, .	1.1	80
39	Ferromagnetic redshift of the optical gap in GdN. Physical Review B, 2007, 76, .	1.1	79
40	First-principles calculations of elasticity, polarization-related properties, and nonlinear optical coefficients in Zn-IV-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>N</mml:mtext><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math Physical Review B, 2009, 79, .	1.1	78
41	UV reflectivity of GaN: Theory and experiment. Physical Review B, 1995, 51, 13516-13532.	1.1	76
42	First-principles study of phonons and related ground-state properties and spectra in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Zn-IV-N</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml: Physical Review B, 2008, 78, .	1.1	76
43	Electronic structure of (diamond C)/(sphalerite BN) (110) interfaces and superlattices. Physical Review B, 1989, 40, 9909-9919.	1.1	74
44	Lattice dynamics in perovskite halides<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="normal">CsSn</mml:mi><mml:msub><mml:mi>X</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>with<mml xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>X</mml:mi><mml:mi>=</mml:mi><mml:mi mathvariant="normal">I</mml:mi><mml:mi>,</mml:mi><mml:mi>Â</mml:mi><mml:mi mathvariant="normal">Br</mml:mi><mml:mi>,</mml:mi><mml:mi>Â</mml:mi><mml:mi mathvariant="nor	1.1	73
45	Tight-binding muffin-tin orbital Green's function method for surface and interface electronic structure calculations. Surface Science, 1986, 178, 256-263.	0.8	72
46	Application of generalized gradient-corrected density functionals to iron. Physical Review B, 1992, 46, 1870-1873.	1.1	72
47	Electronic structure of CrN: A borderline Mott insulator. Physical Review B, 2009, 79, .	1.1	71
48	Single crystal V2O5 and lower oxides. A survey of their electronic, optical, structural, and surface properties. Physica Status Solidi A, 1980, 59, 485-504.	1.7	70
49	Universal Transition State for High-Pressure Zinc Blende to Rocksalt Phase Transitions. Physical Review Letters, 2005, 94, 225501.	2.9	68
50	Interstitial-nitrogen- and oxygen-induced magnetism in Gd-doped GaN. Physical Review B, 2009, 80, .	1.1	65
51	Band structure parameters of wurtzite and zinc-blende GaAs under strain in the GW approximation. Physical Review B, 2011, 84, .	1.1	63
52	Interface-bond-polarity model for semiconductor heterojunction band offsets. Physical Review B, 1990, 41, 2832-2848.	1.1	61
53	Electronic structure of wide-band-gap ternary pnictides with the chalcopyrite structure. Physical Review B, 1994, 49, 4549-4558.	1.1	61
54	Band-structure analysis of the conduction-band mass anisotropy in 6Hand 4HSiC. Physical Review B, 1995, 52, R2249-R2252.	1.1	61

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55	Calculated and measured uv reflectivity of SiC polytypes. Physical Review B, 1994, 50, 10722-10726.	1.1	60
56	First-principles study of the preference for zinc-blende or rocksalt structures in FeN and CoN. Physical Review B, 2004, 70, .	1.1	60
57	Electronic structure of Gd pnictides calculated within theLSDA+Uapproach. Physical Review B, 2006, 74, .	1.1	60
58	Electronic structure and magnetic interactions in MnN andMn3N2. Physical Review B, 2003, 68, .	1.1	57
59	Electronic structure and magnetism in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Bi</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub> xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Bi</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub> Physical Review B, 2008, 78, .	1.1	57
60	Valence band structure of polytypic zinc-blende/wurtzite GaAs nanowires probed by polarization-dependent photoluminescence. Physical Review B, 2012, 85, .	1.1	57
61	Electronic and lattice dynamical properties of IIâ€“Vâ€“N₂ semiconductors. Physica Status Solidi C: Current Topics in Solid State Physics, 2011, 8, 2492-2499.	0.8	56
62	Optical-absorption bands in the 1â€“3 eV range inn-type SiC polytypes. Physical Review B, 1999, 59, 12890-12899.	1.1	54
63	Theory of Semiconductor Heterojunction Valence-Band Offsets: From Supercell Band-Structure Calculations toward a Simple Model. Physical Review Letters, 1988, 61, 1764-1767.	2.9	53
64	Electronic driving force for stacking fault expansion in4Hâ€SiC. Physical Review B, 2006, 73, .	1.1	53
65	Strain effects on the spin-orbit-induced band structure splittings in monolayer MoS<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>and graphene. Physical Review B, 2013, 88, .	1.1	52
66	Unified path for high-pressure transitions of SiC polytypes to the rocksalt structure. Physical Review B, 2003, 68, .	1.1	51
67	Electronic structure and magnetic properties of transition-metal-doped3Cand4Hsilicon carbide. Physical Review B, 2006, 74, .	1.1	50
68	Optical reflectivity of 3C and 4Hâ€SiC polytypes: Theory and experiment. Applied Physics Letters, 1993, 63, 2747-2749.	1.5	49
69	Electronic structure and magnetism of europium chalcogenides in comparison with gadolinium nitride. Journal of Physics Condensed Matter, 2006, 18, 11333-11345.	0.7	49
70	Graphitization Effects on Diamond Surfaces and the Diamond/Graphite Interface. Physica Status Solidi A, 1996, 154, 109-125.	1.7	48
71	Proton irradiation induced defects in Î²-Ga2O3: A combined EPR and theory study. APL Materials, 2019, 7, .	2.2	48
72	Second-harmonic generation in SiC polytypes. Physical Review B, 1998, 57, 9705-9715.	1.1	47

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73	Comparison between experiment and calculated band structures for DyN and SmN. Physical Review B, 2007, 76, .	1.1	47
74	Electronic structure of dense amorphous carbon. Physical Review B, 1994, 49, 11448-11451.	1.1	46
75	Electronic band structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Mg</mml:mi><mml:mo>â^'</mml:mo><mml:mi>IV</mml:mi><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>compounds in the quasiparticle-self-consistent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>approximation. Physical Review B, 2016, 94, .	1.1	46
76	The energy band structure of V2O5. I. Theoretical approach and band calculations. Journal of Physics C: Solid State Physics, 1980, 13, 2485-2500.	1.5	45
77	Valence band effective-mass Hamiltonians for the group-III nitrides from quasiparticle self-consistentGWband structures. Physical Review B, 2012, 85, .	1.1	45
78	Native point defects and doping in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ZnGeN</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>: Physical Review B, 2016, 93, .	1.1	45
79	Mn-dopedScN: A dilute ferromagnetic semiconductor with local exchange coupling. Physical Review B, 2005, 72, .	1.1	44
80	Quasiparticle self-consistent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>of the electronic band structure of bulk and monolayer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">V</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>5</mml:mn></mml:msub></mml:mrow></mml:math>.	1.1	43
81	Disorder effects on the band structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ZnGeN</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>: Role of exchange defects. Physical Review B, 2016, 94, .	1.1	43
82	Pressure dependence of sound velocities in3Câ^'SiCand their relation to the high-pressure phase transition. Physical Review B, 2002, 66, .	1.1	42
83	Electronic structure and magnetism of the semimetals ErAs andErxSc1â^'xAs. Physical Review B, 1994, 50, 7800-7804.	1.1	40
84	X-ray absorption, glancing-angle reflectivity, and theoretical study of the N K- and GaM2,3-edge spectra in GaN. Physical Review B, 1997, 55, 2612-2622.	1.1	40
85	Changes of the geometry and band structure of SiC along the orthorhombic high-pressure transition path between the zinc-blende and rocksalt structures. Physical Review B, 2002, 66, .	1.1	40
86	Stability and half-metallicity of transition metal pnictides in tetrahedrally bonded structures. Physical Review B, 2005, 71, .	1.1	40
87	Vibrational modes in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>ZnGeN</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>: Raman study and theory. Physical Review B, 2008, 77, .	1.1	39
88	Which electronic structure method for the study of defects: A commentary. Physica Status Solidi (B): Basic Research, 2011, 248, 1547-1558.	0.7	39
89	Heteroepitaxy of diamond on c-BN: Growth mechanisms and defect characterization. Journal of Materials Research, 1994, 9, 1849-1865.	1.2	38
90	Structure and phonons ofZnGeN2. Physical Review B, 2005, 72, .	1.1	38

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91	Magnetic exchange interactions in the gadolinium pnictides from first principles. Physical Review B, 2008, 78, .	1.1	38
92	First-principles study of the elasticity, piezoelectricity, and vibrational modes in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LiGaO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:m with ZnO and GaN. Physical Review B, 2010, 81, .	1.1	38
93	Electronic structure of EuN: Growth, spectroscopy, and theory. Physical Review B, 2011, 84, .	1.1	38
94	Computational identification of Ga-vacancy related electron paramagnetic resonance centers in Î²-Ga2O3. Journal of Applied Physics, 2019, 125, .	1.1	38
95	Electronic structure ofZnGeP2:A detailed study of the band structure near the fundamental gap and its associated parameters. Physical Review B, 1999, 60, 8087-8096.	1.1	37
96	Calculated phonon band structure and density of states and interpretation of the Raman spectrum in rocksalt ScN. Physical Review B, 2009, 79, .	1.1	36
97	On the origin of the split-off conduction bands in V2O5. Journal of Physics C: Solid State Physics, 1981, 14, 4785-4795.	1.5	35
98	Magnetic properties of transition-metal nitrides. Journal of Applied Physics, 2005, 97, 10D306.	1.1	35
99	Identification of Raman-active phonon modes in oriented platelets of InN and polycrystalline InN. Solid State Communications, 2000, 114, 355-360.	0.9	33
100	Identification of a N-related shallow acceptor and electron paramagnetic resonance center in ZnO: N<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub><mml:msup><mml:mrow /><mml:mo>+</mml:mo></mml:msup></mml:mrow></mml:math>on the Zn site. Physical Review B, 2013, 87, .	1.1	33
101	Structure and magnetic properties of MnN, CrN, and VN under volume expansion. Physical Review B, 2005, 71, .	1.1	32
102	Vibrational properties of rare-earth nitrides: Raman spectra and theory. Physical Review B, 2009, 79, .	1.1	32
103	All-electron quasiparticle self-consistent <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="italic">GW</mml:mi></mml:math> band structures for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub><m including lattice polarization corrections in different phases. Physical Review Materials, 2018, 2, .	0.9	32
104	Electronic-structure study of the (110) inversion domain boundary in SiC. Physical Review B, 1990, 41, 2948-2958.	1.1	30
105	Noncritically phase-matched second-harmonic-generation chalcopyrites based onCdSiAs2andCdSiP2. Physical Review B, 2004, 70, .	1.1	30
106	V₂O₅: A 2D van der Waals Oxide with Strong In-Plane Electrical and Optical Anisotropy. ACS Applied Materials & Interfaces, 2017, 9, 23949-23956.	4.0	30
107	Internal strain effects on the phase diagram of Ni-Pt alloys. Physical Review B, 1993, 47, 15276-15279.	1.1	29
108	Effects of biaxial strain on stability and half-metallicity of Cr and Mn pnictides and chalcogenides in the zinc-blende structure. Physical Review B, 2005, 72, .	1.1	29

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109	The energy band structure of V2O5. II. Analysis of the theoretical results and comparison with experimental data. Journal of Physics C: Solid State Physics, 1980, 13, 2503-2517.	1.5	28
110	Electronic band structure of graphene from resonant soft x-ray spectroscopy: The role of core-hole effects. Physical Review B, 2012, 86, .	1.1	28
111	Lattice polarization effects on the screened Coulomb interaction <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>W</mml:mi></mml:math> of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml approximation. Physical Review Materials, 2017, 1, .	0.9	28
112	Electronic structure ofBeCN2: A proposed nearly direct wide-band-gap semiconductor. Physical Review B, 1992, 45, 1485-1487.	1.1	27
113	Theoretical study of cation-related point defects inZnGeP2. Physical Review B, 2005, 71, .	1.1	27
114	Quasiparticle self-consistent GW band structure of Î²-Ga2O3 and the anisotropy of the absorption onset. Applied Physics Letters, 2017, 110, .	1.5	27
115	Band Gaps, Bandâ€Offsets, Disorder, Stability Region, and Point Defects in IIâ€IVâ€N₂ Semiconductors. Physica Status Solidi (A) Applications and Materials Science, 2019, 216, 1800875.	0.8	27
116	Spin-dependent resonant tunneling through semimetallic ErAs quantum wells in a magnetic field. Physical Review B, 1996, 53, 3646-3649.	1.1	26
117	Band structure ofCdGeAs2near the fundamental gap. Physical Review B, 2002, 65, .	1.1	26
118	Comment on â€œOrthorhombic Intermediate State in the Zinc Blende to Rocksalt Transformation Path of SiC at High Pressureâ€• Physical Review Letters, 2002, 88, 189601; discussion 189602.	2.9	26
119	Critical evaluation of the LDAâ€‰+â€‰U approach for band gap corrections in point defect calculations: The oxygen vacancy in ZnO case study. Physica Status Solidi (B): Basic Research, 2011, 248, 1043-1051.	0.7	26
120	Phonons and related spectra in bulk and monolayer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>V</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:m mathvariant="normal">O</mml:mi><mml:mn>5</mml:mn></mml:msub></mml:math>. Physical Review B, 2014, 89, .	1.1	26
121	Atomic-resolved depth profile of strain and cation intermixing around LaAlO3/SrTiO3 interfaces. Scientific Reports, 2016, 6, 28118.	1.6	26
122	Distortion modes in halide perovskites: To twist or to stretch, a matter of tolerance and lone pairs. Physical Review Materials, 2018, 2, .	0.9	26
123	Electronic structure of copper/diamond interfaces including effects of interfacial hydrogen. Physica B: Condensed Matter, 1993, 185, 512-527.	1.3	25
124	Deep level defects and cation sublattice disorder in ZnGeN2. Journal of Applied Physics, 2020, 127, .	1.1	24
125	First-principles calculation of the zone center phonons in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Zn</mml:mi><mml:mi mathvariant="normal">Si</mml:mi><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>: Comparison with infrared data. Physical Review B, 2007, 76, .	1.1	23
126	Superparamagnetism in Gd-doped GaN induced by Ga-vacancy clustering. Physical Review B, 2012, 86, .	1.1	23

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127	Electronic structure and total energy of diamond/BeO interfaces. Journal of Materials Research, 1992, 7, 696-705.	1.2	22
128	"Wrong" Bond Interactions at Inversion Domain Boundaries in GaAs. Physical Review Letters, 1992, 68, 1363-1366.	2.9	22
129	Electronic structure of 3C inclusions in 4H SiC. Journal of Applied Physics, 2007, 101, 103711.	1.1	22
130	Calculated interband optical transition spectra of GdN. Physical Review B, 2008, 78, .	1.1	22
131	Electronic band structure information of GdN extracted from x-ray absorption and emission spectroscopy. Applied Physics Letters, 2010, 96, 032101.	1.5	22
132	Optoelectronic Dichotomy of Mixed Halide CH₃NH₃Pb(Br_{1â€“x}Cl_x)₃ Single Crystals: Surface versus Bulk Photoluminescence. Journal of the American Chemical Society, 2018, 140, 11811-11819.	6.6	22
133	Buckled honeycomb antimony: Higher order topological insulator and its relation to the KekulÃ© lattice. Physical Review B, 2020, 102, .	1.1	22
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