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	N₂, NO, and O₂ molecules in LiGaO₂ in both Ga and Li sites and their relation to the vacancies. Journal of Applied Physics, 2022, 131, 145705.	1.1	2
2	Delocalization of dark and bright excitons in flat-band materials and the optical properties of V2O5. Npj Computational Materials, 2022, 8, .	3.5	2
3	Real-space representation of 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> self-energy and its application to defect calculations. Physical Review B, 2022, 105, .	1.1	2
4	Electron microscopy and spectroscopic study of structural changes, electronic properties, and conductivity in annealed <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Li</mml:mi><mml:mi>x</mml:mi></mml:ms Physical Review Materials, 2021, 5, .	0.9	8
5	Topological obstructed atomic limit insulators by annihilating Dirac fermions. Physical Review B, 2021, 103, .	1.1	3
6	Spin-polarized two-dimensional electron/hole gases on LiCoO$_2$ layers.. SciPost Physics, 2021, 10, .	1.5	3
7	Experimental determination of the valence band offsets of ZnGeN₂ and (ZnGe)_{0.94}Ga_{0.12}N₂ with GaN. Journal Physics D: Applied Physics, 2021, 54, 245102.	1.3	6
8	Ultrathin 2D-oxides: A perspective on fabrication, structure, defect, transport, electron, and phonon properties. Journal of Applied Physics, 2021, 129, .	1.1	17
9	Calculated phonon modes, infrared and Raman spectra in orthorhombic Î±â€‰â^'â€‰MoO3 and monolayer MoO3. Journal of Applied Physics, 2021, 130, .	1.1	4
10	Optical response and band structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LiCoO</mml:mi><mml:mn>2</mml:mn></mml:msub></m Including electron-hole interaction effects. Physical Review B, 2021, 104, .	1.1	18
11	<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> band structures and high-pressure phase transitions of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Li</mml:mi><mml:mi>Ga</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Na</mml:mi></mml:mrow></mml:math>	1.1	11
12	Quasiparticle Selfâ€Consistent GW Study of (Ga 1â^' x Al x) 2 O 3 Alloys in Monoclinic and Corundum Structures. Physica Status Solidi (B): Basic Research, 2020, 257, 1900317.	0.7	11
13	Band alignment of III-N, ZnO and IIâ€“IV-N₂ semiconductors from the electron affinity rule. Journal Physics D: Applied Physics, 2020, 53, 015111.	1.3	11
14	Understanding the Crystallographic Phase Relations in Alkaliâ€Trihalogenoâ€Germanates in Terms of Ferroelectric or Antiferroelectric Arrangements of the Tetrahedral GeX₃ Units. Advanced Electronic Materials, 2020, 6, 1900887.	2.6	3
15	Metalâ€“Organic Chemical Vapor Deposition of ZnGeGa₂N₄. Crystal Growth and Design, 2020, 20, 189-196.	1.4	6
16	Effects of the van der Waals Interactions on Structural and Electronic Properties of CH₃NH₃(Pb,Sn)(I,Br,Cl)₃ Halide Perovskites. ACS Omega, 2020, 5, 25723-25732.	1.6	21
17	Buckled honeycomb antimony: Higher order topological insulator and its relation to the KekulÃ© lattice. Physical Review B, 2020, 102, .	1.1	22
18	Electrical Characterization and Charge Transport in Chemically Exfoliated 2D LixCoO2 Nanoflakes. Journal of Physical Chemistry C, 2020, 124, 20693-20700.	1.5	11

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19	Calculated phonon modes, infrared, and Raman spectra in ZnGeGa2N4. Journal of Applied Physics, 2020, 128, 075702.	1.1	4
20	Topological quantum switch and controllable one-dimensional conducting paths in antimonene facilitated by breaking the inversion symmetry. Physical Review B, 2020, 102, .	1.1	1
21	First-principles study of n- and p-type doping opportunities in LiGaO₂. Journal Physics D: Applied Physics, 2020, 53, 274002.	1.3	14
22	Topological band structure transitions and goniopolar transport in honeycomb antimonene as a function of buckling. Physical Review B, 2020, 101, .	1.1	16
23	Deep level defects and cation sublattice disorder in ZnGeN2. Journal of Applied Physics, 2020, 127, .	1.1	24
24	First-principles study of the phonon replicas in the photoluminescence spectrum of 4H -SiC. Physical Review B, 2020, 101, .	1.1	3
25	Candidates for p-type doping of ZnGeN2. Journal of Applied Physics, 2020, 127, 075707.	1.1	9
26	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:n band structure of CrN. Physical Review B, 2020, 101, .	1.1	8
27	Computational study of electron paramagnetic resonance spectra for Li and Ga vacancies in LiGaO₂. Journal Physics D: Applied Physics, 2020, 53, 17LT01.	1.3	7
28	Quasiparticle self-consistent GW energy band calculations for Ge3N4 phases. Physical Review B, 2020, 102, .	1.1	2
29	First-principles calculations of phonon derived Raman and infrared spectra in Be-IV-N₂ compounds. Journal Physics D: Applied Physics, 2019, 52, 385106.	1.3	2
30	First-principles study of point defects in LiGaO2. Journal of Applied Physics, 2019, 126, .	1.1	21
31	Proton irradiation induced defects in Î²-Ga2O3: A combined EPR and theory study. APL Materials, 2019, 7, .	2.2	48
32	Computational identification of Ga-vacancy related electron paramagnetic resonance centers in Î²-Ga2O3. Journal of Applied Physics, 2019, 125, .	1.1	38
33	Computational study of electron paramagnetic resonance parameters for Mg and Zn impurities in Î²-Ga2O3. Applied Physics Letters, 2019, 114, 202102.	1.5	17
34	Quasiparticle self-consistent GW electronic band structures of Be-IV-N₂ compounds. Journal of Physics Condensed Matter, 2019, 31, 335501.	0.7	4
35	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
36	Band Gaps and Stability of CsSiX₃ Halides. Physica Status Solidi (A) Applications and Materials Science, 2019, 216, 1800962.	0.8	5

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37	Instability of the layered orthorhombic post-perovskite phase of SrTiO3 and other candidate orthorhombic phases under pressure. Solid State Communications, 2018, 274, 27-30.	0.9	5
38	Role of the different defects, their population and distribution in the LaAlO3/SrTiO3 heterostructure's behavior. Journal of Applied Physics, 2018, 123, .	1.1	9
39	Ion blocking dip shape analysis around a LaAlO3/SrTiO3 interface. Nuclear Instruments & Methods in Physics Research B, 2018, 423, 67-71.	0.6	2
40	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
41	First-principles calculations of phonons and Raman and infrared spectra in Cd-IV-N2 compounds. Journal of Applied Physics, 2018, 123, .	1.1	8
42	First-principles calculations of elastic and piezoelectric constants and spontaneous polarization in Cd-IV-N2 compounds. Journal of Applied Physics, 2018, 124, .	1.1	4
43	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
44	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
45	Ordering in the mixed <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>-/ -GaN alloy system: Crystal structures and band structures of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>ZnGeGa</mml:mi><mml:mn>2</mml:mn><mml:mi mathvariant="normal">N</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> from first principles. Physical Review Materials, 2018, 2, .	0.9	11
46	First-principles calculations of second-order nonlinear optical coefficients in the static limit and Pockels coefficients in III-N and IIâ^'IVâ^'N2 compounds. Physical Review Materials, 2018, 2, .	0.9	3
47	Core-level binding energy shifts as a tool to study surface processes on LaAlO 3 /SrTiO 3. Journal of Electron Spectroscopy and Related Phenomena, 2017, 218, 21-29.	0.8	17
48	Quasiparticle self-consistent GW band structure of Î²-Ga2O3 and the anisotropy of the absorption onset. Applied Physics Letters, 2017, 110, .	1.5	27
49	Raman study of the vibrational modes in ZnGeN2 (0001). Journal of Applied Physics, 2017, 121, .	1.1	9
50	Carrier-controlled anomalous Hall effect in an intrinsic ferromagnetic semiconductor. Physical Review B, 2017, 96, .	1.1	14
51	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
52	Zone-center phonons in yellow phase <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="bold">CsSnI</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review Materials, 2017, 1, .	0.9	2
53	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></mm band structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>Cd-IV-N</mml:mtext><mml:mn>2</mml:mn></mml:m 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	0.9	15
54	<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:m approximation. Physical Review Materials, 2017, 1, .	0.9	28

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55	Native interstitial defects 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> Physical Review Materials, 2017, 1, .	0.9	7
56	Atomic-resolved depth profile of strain and cation intermixing around LaAlO3/SrTiO3 interfaces. Scientific Reports, 2016, 6, 28118.	1.6	26
57	Vibrational modes in the Pmc21 structure of ZnGeN2. Solid State Communications, 2016, 233, 46-49.	0.9	6
58	Vibrational spectra and nonlinear optical coefficients of rhombohedral<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>CsGe</mml:mi><mml:msub><mml:mi>X</mml:mi><mml: compounds with<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>X</mml:mi><mml:mo>=</mml:mo><mml:mi mathvariant="normal">I</mml:mi></mml:mrow></mml:math>. Br, Cl. Physical Review B, 2016, 94, .	1.1	15
59	<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> 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: Physical Review B, 2016, 94, .	1.1	46
60	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> Physical Review B, 2016, 93, .	1.1	45
61	Publisher's Note: Effects of structural relaxation, interdiffusion, and surface termination on two-dimensional electron gas formation at theLaAlO3/SrTiO3(001) interface [Phys. Rev. B92, 155416 (2015)]. Physical Review B, 2016, 93, .	1.1	0
62	Electronic band structure trends of perovskite halides: Beyond Pb and Sn to Ge and Si. Physical Review B, 2016, 93, .	1.1	130
63	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> Role of exchange defects. Physical Review B, 2016, 94, .	1.1	43
64	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
65	Fully opposite spin polarization of electron and hole bands in DyN and related band structures of GdN and HoN. Physical Review B, 2015, 92, .	1.1	5
66	Systematic study of the exchange interactions in Gd-doped GaN containing N interstitials, O interstitials, or Ga vacancies. Physical Review B, 2015, 92, .	1.1	16
67	Electronic and magnetic properties of electrondoped<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>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>NaV</mml:mi><mml:mn>2</mml:mn></mml: Physical Review B,	1.1	9
68	Effects of structural relaxation, interdiffusion, and surface termination on two-dimensional electron gas formation at the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>LaAlO</mml:mi><mml:mn>3</mml:mn></mml: interface. Physical Review B, 2015, 92, .	1.1	17
69	<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: 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
70	First-principles calculations of phonons and Raman spectra in monoclinic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="normal">CsSnCl</mml:mi><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2015, 91, .	1.1	13
71	Publisher's Note: Phonons and related spectra in bulk and monolayerV2O5[Phys. Rev. B89, 045109 (2014)]. Physical Review B, 2014, 89, .	1.1	0
72	Theory of light emission polarization reversal in zinc-blende and wurtzite nanowires. Physical Review B, 2014, 89, .	1.1	9

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73	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
74	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	1.1	73
75	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
76	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
77	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:mrow	1.1	404
78	Electronic structure of defects and doping in ZnO: Oxygen vacancy and nitrogen doping. Physica Status Solidi (B): Basic Research, 2013, 250, 2091-2101.	0.7	21
79	Rare-earth mononitrides. Progress in Materials Science, 2013, 58, 1316-1360.	16.0	124
80	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
81	Electronic structure of defects and doping in ZnO: Oxygen vacancy and nitrogen doping. Physica Status Solidi (B): Basic Research, 2013, 250, .	0.7	18
82	Heterovalent ternary II-IV-N2 compounds: perspectives for a new class of wide-band-gap nitrides. , 2013, , 519-585.		16
83	Nitrogen pair â˜ hydrogen complexes in ZnO and p-type doping.. Materials Research Society Symposia Proceedings, 2012, 1394, 27.	0.1	5
84	Superparamagnetism in Gd-doped GaN induced by Ga-vacancy clustering. Physical Review B, 2012, 86, .	1.1	23
85	Single well or double well: First-principles study of 8<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>H</mml:mi></mml:math>and 3<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>C</mml:mi></mml:math>inclusions in the 4<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>H</mml:mi></mml:math>	1.1	6
86	Valence band effective-mass Hamiltonians for the group-III nitrides from quasiparticle self-consistentGWband structures. Physical Review B, 2012, 85, .	1.1	45
87	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
88	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
89	Valence band structure of polytypic zinc-blende/wurtzite GaAs nanowires probed by polarization-dependent photoluminescence. Physical Review B, 2012, 85, .	1.1	57
90	First-principles calculation of resonant x-ray emission spectra applied to ZnO. Physical Review B, 2011, 83, .	1.1	8

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91	Band structure parameters of wurtzite and zinc-blende GaAs under strain in the GW approximation. Physical Review B, 2011, 84, .	1.1	63
92	Which electronic structure method for the study of defects: A commentary. Physica Status Solidi (B): Basic Research, 2011, 248, 1547-1558.	0.7	39
93	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
94	Electronic and lattice dynamical properties of IIâ€“IVâ€“N₂ semiconductors. Physica Status Solidi C: Current Topics in Solid State Physics, 2011, 8, 2492-2499.	0.8	56
95	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
96	Calculated x-ray linear dichroism spectra for Gd-doped GaN. Physical Review B, 2011, 84, .	1.1	1
97	Electronic structure of EuN: Growth, spectroscopy, and theory. Physical Review B, 2011, 84, .	1.1	38
98	Site Dependence of Electronic Structure of Gd Impurities in GaN. Materials Research Society Symposia Proceedings, 2011, 1290, 1.	0.1	2
99	First-principles Study of Nitrogen Vacancies in GdN. Materials Research Society Symposia Proceedings, 2011, 1290, 1.	0.1	21
100	Electronic structure, doping, and lattice dynamics of LiGaO 2. Proceedings of SPIE, 2011, , .	0.8	6
101	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
102	Electronic band structure information of GdN extracted from x-ray absorption and emission spectroscopy. Applied Physics Letters, 2010, 96, 032101.	1.5	22
103	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:msub></mml:mrow></mml:math>with ZnO and GaN. Physical Review B, 2010, 81, .	1.1	38
104	First-principles study of oxygen vacancies in<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:msub></mml:mrow></mml:math>Physical Review B, 2010, 81, .	1.1	13
105	Interstitial-nitrogen- and oxygen-induced magnetism in Gd-doped GaN. Physical Review B, 2009, 80, .	1.1	65
106	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
107	Computational study of phonon modes in short-period AlN/GaN superlattices. Physical Review B, 2009, 80, .	1.1	14
108	Vibrational properties of rare-earth nitrides: Raman spectra and theory. Physical Review B, 2009, 79, .	1.1	32

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