

Walter R L Lambrecht

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

265
papers

11,620
citations

54
h-index

99
g-index

281
ext. papers

12,575
ext. citations

3.6
avg, IF

6.69
L-index

#	Paper	IF	Citations
265	N ₂ , NO, and O ₂ molecules in LiGaO ₂ in both Ga and Li sites and their relation to the vacancies. <i>Journal of Applied Physics</i> , 2022 , 131, 145705	2.5	0
264	Spin-polarized two-dimensional electron/hole gases on LiCoO ₂ layers.. <i>SciPost Physics</i> , 2021 , 10,	6.1	2
263	Experimental determination of the valence band offsets of ZnGeN ₂ and (ZnGe) _{0.94} Ga _{0.12} N ₂ with GaN. <i>Journal Physics D: Applied Physics</i> , 2021 , 54, 245102	3	2
262	Ultrathin 2D-oxides: A perspective on fabrication, structure, defect, transport, electron, and phonon properties. <i>Journal of Applied Physics</i> , 2021 , 129, 220903	2.5	4
261	Electron microscopy and spectroscopic study of structural changes, electronic properties, and conductivity in annealed Li _x CoO ₂ . <i>Physical Review Materials</i> , 2021 , 5,	3.2	3
260	Calculated phonon modes, infrared and Raman spectra in orthorhombic $\sqrt{3}\times\sqrt{3}$ MoO ₃ and monolayer MoO ₃ . <i>Journal of Applied Physics</i> , 2021 , 130, 104302	2.5	
259	Optical response and band structure of LiCoO ₂ including electron-hole interaction effects. <i>Physical Review B</i> , 2021 , 104,	3.3	3
258	Quasiparticle self-consistent GW band structures and high-pressure phase transitions of LiGaO ₂ and NaGaO ₂ . <i>Physical Review B</i> , 2021 , 103,	3.3	3
257	Topological quantum switch and controllable one-dimensional conducting paths in antimonene facilitated by breaking the inversion symmetry. <i>Physical Review B</i> , 2020 , 102,	3.3	1
256	First-principles study of n- and p-type doping opportunities in LiGaO ₂ . <i>Journal Physics D: Applied Physics</i> , 2020 , 53, 274002	3	6
255	Topological band structure transitions and goniopolar transport in honeycomb antimonene as a function of buckling. <i>Physical Review B</i> , 2020 , 101,	3.3	6
254	Deep level defects and cation sublattice disorder in ZnGeN ₂ . <i>Journal of Applied Physics</i> , 2020 , 127, 1357035	2.5	12
253	First-principles study of the phonon replicas in the photoluminescence spectrum of 4H-SiC. <i>Physical Review B</i> , 2020 , 101,	3.3	1
252	Candidates for p-type doping of ZnGeN ₂ . <i>Journal of Applied Physics</i> , 2020 , 127, 075707	2.5	4
251	Quasiparticle self-consistent GW band structure of CrN. <i>Physical Review B</i> , 2020 , 101,	3.3	4
250	Computational study of electron paramagnetic resonance spectra for Li and Ga vacancies in LiGaO ₂ . <i>Journal Physics D: Applied Physics</i> , 2020 , 53, 17LT01	3	1
249	Quasiparticle self-consistent GW energy band calculations for Ge ₃ N ₄ phases. <i>Physical Review B</i> , 2020 , 102,	3.3	2

248	Band alignment of III-N, ZnO and IIIV-N2 semiconductors from the electron affinity rule. <i>Journal Physics D: Applied Physics</i> , 2020 , 53, 015111	3	6
247	Understanding the Crystallographic Phase Relations in Alkali-Trihalogeno-Germanates in Terms of Ferroelectric or Antiferroelectric Arrangements of the Tetrahedral GeX3 Units. <i>Advanced Electronic Materials</i> , 2020 , 6, 1900887	6.4	0
246	MetalOrganic Chemical Vapor Deposition of ZnGeGa2N4. <i>Crystal Growth and Design</i> , 2020 , 20, 189-196	3.5	4
245	Effects of the van der Waals Interactions on Structural and Electronic Properties of CHNH(Pb,Sn)(I,Br,Cl) Halide Perovskites. <i>ACS Omega</i> , 2020 , 5, 25723-25732	3.9	4
244	Buckled honeycomb antimony: Higher order topological insulator and its relation to the Kekul� lattice. <i>Physical Review B</i> , 2020 , 102,	3.3	6
243	Electrical Characterization and Charge Transport in Chemically Exfoliated 2D Li _x CoO ₂ Nanoflakes. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 20693-20700	3.8	6
242	Calculated phonon modes, infrared, and Raman spectra in ZnGeGa2N4. <i>Journal of Applied Physics</i> , 2020 , 128, 075702	2.5	0
241	Quasiparticle Self-Consistent GW Study of (Ga _{1-x} Al _x) ₂ O ₃ Alloys in Monoclinic and Corundum Structures. <i>Physica Status Solidi (B): Basic Research</i> , 2020 , 257, 1900317	1.3	4
240	Proton irradiation induced defects in Ga ₂ O ₃ : A combined EPR and theory study. <i>APL Materials</i> , 2019 , 7, 022521	5.7	33
239	Computational identification of Ga-vacancy related electron paramagnetic resonance centers in Ga ₂ O ₃ . <i>Journal of Applied Physics</i> , 2019 , 125, 185701	2.5	22
238	Computational study of electron paramagnetic resonance parameters for Mg and Zn impurities in Ga ₂ O ₃ . <i>Applied Physics Letters</i> , 2019 , 114, 202102	3.4	12
237	Quasiparticle self-consistent GW electronic band structures of Be-IV-N compounds. <i>Journal of Physics Condensed Matter</i> , 2019 , 31, 335501	1.8	2
236	Band Gaps, Band-Offsets, Disorder, Stability Region, and Point Defects in II-IV-N ₂ Semiconductors. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2019 , 216, 1800875	1.6	16
235	Band Gaps and Stability of CsSiX ₃ Halides. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2019 , 216, 1800962	1.6	2
234	First-principles calculations of phonon derived Raman and infrared spectra in Be-IV-N ₂ compounds. <i>Journal Physics D: Applied Physics</i> , 2019 , 52, 385106	3	2
233	First-principles study of point defects in LiGaO ₂ . <i>Journal of Applied Physics</i> , 2019 , 126, 155703	2.5	8
232	Instability of the layered orthorhombic post-perovskite phase of SrTiO ₃ and other candidate orthorhombic phases under pressure. <i>Solid State Communications</i> , 2018 , 274, 27-30	1.6	3
231	Role of the different defects, their population and distribution in the LaAlO ₃ /SrTiO ₃ heterostructure's behavior. <i>Journal of Applied Physics</i> , 2018 , 123, 155304	2.5	6

230	Ion blocking dip shape analysis around a LaAlO ₃ /SrTiO ₃ interface. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2018 , 423, 67-71	1.2	2
229	First-principles calculations of elastic and piezoelectric constants and spontaneous polarization in Cd-IV-N ₂ compounds. <i>Journal of Applied Physics</i> , 2018 , 124, 055705	2.5	2
228	All-electron quasiparticle self-consistent GW band structures for SrTiO ₃ including lattice polarization corrections in different phases. <i>Physical Review Materials</i> , 2018 , 2,	3.2	21
227	Distortion modes in halide perovskites: To twist or to stretch, a matter of tolerance and lone pairs. <i>Physical Review Materials</i> , 2018 , 2,	3.2	15
226	Ordering in the mixed ZnGeN ₂ -GaN alloy system: Crystal structures and band structures of ZnGeGa ₂ N ₄ from first principles. <i>Physical Review Materials</i> , 2018 , 2,	3.2	9
225	First-principles calculations of second-order nonlinear optical coefficients in the static limit and Pockels coefficients in III-N and III-V-N ₂ compounds. <i>Physical Review Materials</i> , 2018 , 2,	3.2	2
224	Optoelectronic Dichotomy of Mixed Halide CH ₃ NHPb(BrCl) Single Crystals: Surface versus Bulk Photoluminescence. <i>Journal of the American Chemical Society</i> , 2018 , 140, 11811-11819	16.4	18
223	First-principles calculations of phonons and Raman and infrared spectra in Cd-IV-N ₂ compounds. <i>Journal of Applied Physics</i> , 2018 , 123, 205701	2.5	7
222	Core-level binding energy shifts as a tool to study surface processes on LaAlO ₃ /SrTiO ₃ . <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2017 , 218, 21-29	1.7	12
221	Quasiparticle self-consistent GW band structure of Ga ₂ O ₃ and the anisotropy of the absorption onset. <i>Applied Physics Letters</i> , 2017 , 110, 132103	3.4	22
220	Raman study of the vibrational modes in ZnGeN ₂ (0001). <i>Journal of Applied Physics</i> , 2017 , 121, 055704	2.5	9
219	Carrier-controlled anomalous Hall effect in an intrinsic ferromagnetic semiconductor. <i>Physical Review B</i> , 2017 , 96,	3.3	12
218	VO: A 2D van der Waals Oxide with Strong In-Plane Electrical and Optical Anisotropy. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 23949-23956	9.5	23
217	Zone-center phonons in yellow phase CsSnI ₃ . <i>Physical Review Materials</i> , 2017 , 1,	3.2	2
216	Quasiparticle self-consistent GW electronic band structure of Cd-IV-N ₂ compounds. <i>Physical Review Materials</i> , 2017 , 1,	3.2	12
215	Lattice polarization effects on the screened Coulomb interaction W of the GW approximation. <i>Physical Review Materials</i> , 2017 , 1,	3.2	25
214	Native interstitial defects in ZnGeN ₂ . <i>Physical Review Materials</i> , 2017 , 1,	3.2	7
213	Vibrational spectra and nonlinear optical coefficients of rhombohedral CsGeX ₃ halide compounds with X=I, Br, Cl. <i>Physical Review B</i> , 2016 , 94,	3.3	11

212	Electronic band structure of $MgMn_2$ compounds in the quasiparticle-self-consistent GW approximation. <i>Physical Review B</i> , 2016 , 94,	3-3	39
211	Native point defects and doping in $ZnGeN_2$. <i>Physical Review B</i> , 2016 , 93,	3-3	38
210	Electronic band structure trends of perovskite halides: Beyond Pb and Sn to Ge and Si. <i>Physical Review B</i> , 2016 , 93,	3-3	86
209	Disorder effects on the band structure of $ZnGeN_2$: Role of exchange defects. <i>Physical Review B</i> , 2016 , 94,	3-3	31
208	Atomic-resolved depth profile of strain and cation intermixing around $LaAlO_3/SrTiO_3$ interfaces. <i>Scientific Reports</i> , 2016 , 6, 28118	4-9	22
207	Vibrational modes in the $Pmc2_1$ structure of $ZnGeN_2$. <i>Solid State Communications</i> , 2016 , 233, 46-49	1-6	6
206	First-principles calculations of phonons and Raman spectra in monoclinic $CsSnCl_3$. <i>Physical Review B</i> , 2015 , 91,	3-3	9
205	Charge-neutral disorder and polytypes in heterovalent wurtzite-based ternary semiconductors: The importance of the octet rule. <i>Physical Review B</i> , 2015 , 91,	3-3	76
204	Fully opposite spin polarization of electron and hole bands in DyN and related band structures of GdN and HoN . <i>Physical Review B</i> , 2015 , 92,	3-3	3
203	Systematic study of the exchange interactions in Gd-doped GaN containing N interstitials, O interstitials, or Ga vacancies. <i>Physical Review B</i> , 2015 , 92,	3-3	14
202	Electronic and magnetic properties of electron-doped V_2O_5 and NaV_2O_5 . <i>Physical Review B</i> , 2015 , 92,	3-3	5
201	Effects of structural relaxation, interdiffusion, and surface termination on two-dimensional electron gas formation at the $LaAlO_3/SrTiO_3$ (001) interface. <i>Physical Review B</i> , 2015 , 92,	3-3	16
200	Quasiparticle self-consistent GW calculations of the electronic band structure of bulk and monolayer V_2O_5 . <i>Physical Review B</i> , 2015 , 91,	3-3	33
199	Theory of light emission polarization reversal in zinc-blende and wurtzite nanowires. <i>Physical Review B</i> , 2014 , 89,	3-3	7
198	Phonons and related spectra in bulk and monolayer V_2O_5 . <i>Physical Review B</i> , 2014 , 89,	3-3	22
197	Lattice dynamics in perovskite halides $CsSnX_3$ with $X=I, Br, Cl$. <i>Physical Review B</i> , 2014 , 90,	3-3	54
196	Band offsets between $ZnGeN_2$, GaN, ZnO, and $ZnSnN_2$ and their potential impact for solar cells. <i>Physical Review B</i> , 2013 , 88,	3-3	72
195	Strain effects on the spin-orbit-induced band structure splittings in monolayer MoS_2 and graphene. <i>Physical Review B</i> , 2013 , 88,	3-3	40

194	Electronic band structure, phonons, and exciton binding energies of halide perovskites CsSnCl ₃ , CsSnBr ₃ , and CsSnI ₃ . <i>Physical Review B</i> , 2013 , 88,	3-3	312
193	Electronic structure of defects and doping in ZnO: Oxygen vacancy and nitrogen doping. <i>Physica Status Solidi (B): Basic Research</i> , 2013 , 250, 2091-2101	1-3	16
192	Rare-earth mononitrides. <i>Progress in Materials Science</i> , 2013 , 58, 1316-1360	42.2	93
191	Identification of a N-related shallow acceptor and electron paramagnetic resonance center in ZnO: N ₂ ⁺ on the Zn site. <i>Physical Review B</i> , 2013 , 87,	3-3	27
190	Electronic structure of defects and doping in ZnO: Oxygen vacancy and nitrogen doping. <i>Physica Status Solidi (B): Basic Research</i> , 2013 , 250, n/a-n/a	1-3	18
189	Heterovalent ternary II-IV-N ₂ compounds: perspectives for a new class of wide-band-gap nitrides 2013 , 519-585		14
188	Valence band effective-mass Hamiltonians for the group-III nitrides from quasiparticle self-consistent GW band structures. <i>Physical Review B</i> , 2012 , 85,	3-3	35
187	Electronic band structure of graphene from resonant soft x-ray spectroscopy: The role of core-hole effects. <i>Physical Review B</i> , 2012 , 86,	3-3	25
186	Quasiparticle band structure calculation of monolayer, bilayer, and bulk MoS ₂ . <i>Physical Review B</i> , 2012 , 85,	3-3	980
185	GaAs Nanowires: A New Place to Explore Polytype Physics. <i>Materials Science Forum</i> , 2012 , 717-720, 565-568		1
184	Valence band structure of polytypic zinc-blende/wurtzite GaAs nanowires probed by polarization-dependent photoluminescence. <i>Physical Review B</i> , 2012 , 85,	3-3	53
183	Nitrogen pair/hydrogen complexes in ZnO and p-type doping.. <i>Materials Research Society Symposia Proceedings</i> , 2012 , 1394, 27		4
182	Superparamagnetism in Gd-doped GaN induced by Ga-vacancy clustering. <i>Physical Review B</i> , 2012 , 86,	3-3	22
181	Single well or double well: First-principles study of 8H and 3C inclusions in the 4H SiC polytype. <i>Physical Review B</i> , 2012 , 85,	3-3	3
180	CdGeN ₂ and ZnGe _{0.5} Sn _{0.5} N ₂ : Two New Nitride Semiconductors with Band Gaps in the Blue-Green. <i>Materials Science Forum</i> , 2012 , 717-720, 1331-1334	0-4	4
179	First-principles calculation of resonant x-ray emission spectra applied to ZnO. <i>Physical Review B</i> , 2011 , 83,	3-3	5
178	Band structure parameters of wurtzite and zinc-blende GaAs under strain in the GW approximation. <i>Physical Review B</i> , 2011 , 84,	3-3	58
177	Critical Evaluation of the LDA + U Approach for Band Gap Corrections in Point Defect Calculations: The Oxygen Vacancy in ZnO Case Study 2011 , 165-181		

176	Which Electronic Structure Method for The Study of Defects: A Commentary 2011 , 359-379		
175	Which electronic structure method for the study of defects: A commentary. <i>Physica Status Solidi (B): Basic Research</i> , 2011 , 248, 1547-1558	1-3	35
174	Critical evaluation of the LDA + U approach for band gap corrections in point defect calculations: The oxygen vacancy in ZnO case study. <i>Physica Status Solidi (B): Basic Research</i> , 2011 , 248, 1043-1051	1-3	24
173	Electronic and lattice dynamical properties of II-IV-N ₂ semiconductors. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2011 , 8, 2492-2499		45
172	Quasiparticle band structure of Zn-IV-N ₂ compounds. <i>Physical Review B</i> , 2011 , 84,	3-3	109
171	Calculated x-ray linear dichroism spectra for Gd-doped GaN. <i>Physical Review B</i> , 2011 , 84,	3-3	1
170	Electronic structure of EuN: Growth, spectroscopy, and theory. <i>Physical Review B</i> , 2011 , 84,	3-3	31
169	Site Dependence of Electronic Structure of Gd Impurities in GaN. <i>Materials Research Society Symposia Proceedings</i> , 2011 , 1290, 1		2
168	First-principles Study of Nitrogen Vacancies in GdN. <i>Materials Research Society Symposia Proceedings</i> , 2011 , 1290, 1		19
167	Electronic structure, doping, and lattice dynamics of LiGaO ₂ 2011 ,		5
166	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. <i>Physical Review B</i> , 2010 , 82,	3-3	78
165	Electronic band structure information of GdN extracted from x-ray absorption and emission spectroscopy. <i>Applied Physics Letters</i> , 2010 , 96, 032101	3-4	18
164	First-principles study of the elasticity, piezoelectricity, and vibrational modes in LiGaO ₂ compared with ZnO and GaN. <i>Physical Review B</i> , 2010 , 81,	3-3	33
163	First-principles study of oxygen vacancies in Mg _x Zn _{1-x} O alloys. <i>Physical Review B</i> , 2010 , 81,	3-3	12
162	Interstitial-nitrogen- and oxygen-induced magnetism in Gd-doped GaN. <i>Physical Review B</i> , 2009 , 80,	3-3	59
161	First-principles calculations of elasticity, polarization-related properties, and nonlinear optical coefficients in Zn-IV-N ₂ compounds. <i>Physical Review B</i> , 2009 , 79,	3-3	61
160	Computational study of phonon modes in short-period AlN/GaN superlattices. <i>Physical Review B</i> , 2009 , 80,	3-3	12
159	Vibrational properties of rare-earth nitrides: Raman spectra and theory. <i>Physical Review B</i> , 2009 , 79,	3-3	21

158	Bond lengths, phase stability, and band gaps in $\text{Mg}_x\text{Zn}_{1-x}\text{O}$ alloys. <i>Journal of Vacuum Science & Technology B</i> , 2009 , 27, 1717		3
157	Calculated phonon band structure and density of states and interpretation of the Raman spectrum in rocksalt ScN. <i>Physical Review B</i> , 2009 , 79,	3-3	31
156	Electronic structure of CrN: A borderline Mott insulator. <i>Physical Review B</i> , 2009 , 79,	3-3	62
155	Jahn-Teller Distortion of the Zinc Vacancy in ZnGeP ₂ . <i>Chinese Physics Letters</i> , 2008 , 25, 1075-1078	1.8	2
154	Calculated interband optical transition spectra of GdN. <i>Physical Review B</i> , 2008 , 78,	3-3	19
153	Vibrational modes in ZnGeN ₂ : Raman study and theory. <i>Physical Review B</i> , 2008 , 77,	3-3	34
152	First-principles study of phonons and related ground-state properties and spectra in Zn-IV-N ₂ compounds. <i>Physical Review B</i> , 2008 , 78,	3-3	61
151	Linear response theoretical study of the exchange interactions in Mn-doped ScN: Effects of disorder, band gap, and doping. <i>Physical Review B</i> , 2008 , 77,	3-3	15
150	Magnetic exchange interactions in the gadolinium pnictides from first principles. <i>Physical Review B</i> , 2008 , 78,	3-3	35
149	First-principles calculation of the O vacancy in ZnO: A self-consistent gap-corrected approach. <i>Physical Review B</i> , 2008 , 77,	3-3	123
148	First-principles study of native defects in CdGeAs ₂ . <i>Physical Review B</i> , 2008 , 78,	3-3	10
147	Electronic structure and magnetism in Bi ₂ Te ₃ , Bi ₂ Se ₃ , and Sb ₂ Te ₃ doped with transition metals (Ti/N). <i>Physical Review B</i> , 2008 , 78,	3-3	53
146	Effects of vacancies and impurities on the relative stability of rocksalt and zincblende structures for MnN. <i>Physical Review B</i> , 2007 , 76,	3-3	9
145	Electronic and crystal structure of Cu ₂ S: Full-potential electronic structure calculations. <i>Physical Review B</i> , 2007 , 76,	3-3	202
144	Electronic structure of 3C inclusions in 4H SiC. <i>Journal of Applied Physics</i> , 2007 , 101, 103711	2.5	20
143	First-principles calculation of the zone center phonons in ZnSiN ₂ : Comparison with infrared data. <i>Physical Review B</i> , 2007 , 76,	3-3	21
142	Comparison between experiment and calculated band structures for DyN and SmN. <i>Physical Review B</i> , 2007 , 76,	3-3	40
141	Ferromagnetic redshift of the optical gap in GdN. <i>Physical Review B</i> , 2007 , 76,	3-3	67

140	Large band-gap bowing in $\text{Cu}_{1-x}\text{Ag}_x\text{GaS}_2$ chalcopyrite semiconductors and its effect on optical parameters. <i>Physical Review B</i> , 2007 , 76,	3.3	4
139	Electronic structure of rare-earth nitrides using the LSDA+U approach: Importance of allowing 4f orbitals to break the cubic crystal symmetry. <i>Physical Review B</i> , 2007 , 75,	3.3	270
138	Band-gap bowing in $\text{AgGa}(\text{Se}_{1-x}\text{Te}_x)_2$ and its effect on the second-order response coefficient and refractive indices. <i>Physical Review B</i> , 2007 , 76,	3.3	6
137	Stacking Faults and 3C Quantum Wells in Hexagonal SiC Polytypes. <i>Materials Science Forum</i> , 2006 , 527-529, 351-354	0.4	2
136	Gadolinium and Oxygen co-doping of Gallium Nitride: an LSDA + U study. <i>Materials Research Society Symposia Proceedings</i> , 2006 , 955, 1		
135	Electronic structure and magnetic properties of transition-metal-doped 3C and 4H silicon carbide. <i>Physical Review B</i> , 2006 , 74,	3.3	45
134	Electronic structure of Gd pnictides calculated within the LSDA+U approach. <i>Physical Review B</i> , 2006 , 74,	3.3	52
133	Theoretical study of the phosphorus vacancy in ZnGeP_2 . <i>Physical Review B</i> , 2006 , 73,	3.3	16
132	Electronic driving force for stacking fault expansion in 4H-SiC. <i>Physical Review B</i> , 2006 , 73,	3.3	49
131	Electronic structure and magnetism of europium chalcogenides in comparison with gadolinium nitride. <i>Journal of Physics Condensed Matter</i> , 2006 , 18, 11333-11345	1.8	40
130	Electronic Structure and Magnetic Properties of Transition Metal Doped Silicon Carbide in Different Polytypes. <i>Materials Science Forum</i> , 2006 , 527-529, 641-646	0.4	1
129	Mn-doped ScN: A dilute ferromagnetic semiconductor with local exchange coupling. <i>Physical Review B</i> , 2005 , 72,	3.3	41
128	Magnetic properties of transition-metal nitrides. <i>Journal of Applied Physics</i> , 2005 , 97, 10D306	2.5	31
127	Structure and magnetic properties of MnN, CrN, and VN under volume expansion. <i>Physical Review B</i> , 2005 , 71,	3.3	28
126	Optical conductivity and x-ray absorption and emission study of the band structure of MnN films. <i>Physical Review B</i> , 2005 , 72,	3.3	9
125	Recent advances in atomic-scale spin-polarized scanning tunneling microscopy. <i>Microscopy Research and Technique</i> , 2005 , 66, 72-84	2.8	7
124	Crystal structure, electronic structure and magnetism of transition metal nitrides. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2005 , 2, 2516-2519		14
123	First-principles study of the structural and magnetic properties of iron indium nitride. <i>Journal of Applied Physics</i> , 2005 , 97, 10D309	2.5	3

122	Electronic structure and magnetic properties of Mn ₃ GaN precipitates in Ga _{1-x} MnxN. <i>Physical Review B</i> , 2005 , 72,	3-3	18
121	Theoretical study of cation-related point defects in ZnGeP ₂ . <i>Physical Review B</i> , 2005 , 71,	3-3	23
120	Stability and half-metallicity of transition metal pnictides in tetrahedrally bonded structures. <i>Physical Review B</i> , 2005 , 71,	3-3	37
119	Universal transition state for high-pressure zinc blende to rocksalt phase transitions. <i>Physical Review Letters</i> , 2005 , 94, 225501	7-4	64
118	Structure and phonons of ZnGeN ₂ . <i>Physical Review B</i> , 2005 , 72,	3-3	36
117	The effects of biaxial strain on stability and half-metallicity of zinc blende CrSb. <i>Journal of Applied Physics</i> , 2005 , 97, 10C304	2-5	5
116	Effects of biaxial strain on stability and half-metallicity of Cr and Mn pnictides and chalcogenides in the zinc-blende structure. <i>Physical Review B</i> , 2005 , 72,	3-3	28
115	Noncritically phase-matched second-harmonic-generation chalcopyrites based on CdSiAs ₂ and CdSiP ₂ . <i>Physical Review B</i> , 2004 , 70,	3-3	25
114	Electronic band structure of ordered vacancy defect chalcopyrite compounds with formula A ₂ B ₂ C ₄ . <i>Physical Review B</i> , 2004 , 69,	3-3	79
113	First-principles study of the preference for zinc-blende or rocksalt structures in FeN and CoN. <i>Physical Review B</i> , 2004 , 70,	3-3	56
112	First-principles calculations of second-order optical response functions in chalcopyrite semiconductors. <i>Journal of Physics and Chemistry of Solids</i> , 2003 , 64, 1615-1619	3-9	17
111	Electronic structure of thin heterocrystalline superlattices in SiC and AlN. <i>Physical Review B</i> , 2003 , 68,	3-3	19
110	Magnetic properties of substitutional 3d transition metal impurities in silicon carbide. <i>Physical Review B</i> , 2003 , 68,	3-3	71
109	Electronic Structure of Native Point Defects in ZnGeP ₂ . <i>Materials Research Society Symposia Proceedings</i> , 2003 , 799, 203		
108	Unified path for high-pressure transitions of SiC polytypes to the rocksalt structure. <i>Physical Review B</i> , 2003 , 68,	3-3	49
107	Electronic structure and magnetic interactions in MnN and Mn ₃ N ₂ . <i>Physical Review B</i> , 2003 , 68,	3-3	55
106	Anisotropy of UV-reflectivity in wurtzite crystals: a comparison between GaN and CdSe. <i>Solid State Communications</i> , 2002 , 121, 549-554	1-6	10
105	Atomic-scale spin-polarized scanning tunneling microscopy applied to Mn ₃ N ₂ (010). <i>Physical Review Letters</i> , 2002 , 89, 226101	7-4	70

104	Band structure of CdGeAs ₂ near the fundamental gap. <i>Physical Review B</i> , 2002 , 65,	3-3	24
103	Changes of the geometry and band structure of SiC along the orthorhombic high-pressure transition path between the zinc-blende and rocksalt structures. <i>Physical Review B</i> , 2002 , 66,	3-3	39
102	Pressure dependence of sound velocities in 3C-SiC and their relation to the high-pressure phase transition. <i>Physical Review B</i> , 2002 , 66,	3-3	37
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