Walter R L Lambrecht

List of Publications by Citations

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	Quasiparticle band structure calculation of monolayer, bilayer, and bulk MoS2. *Physical Review B*, **2012**, 85,	3.3	980
264	Elastic constants and related properties of tetrahedrally bonded BN, AlN, GaN, and InN. *Physical Review B*, **1996**, 53, 16310-16326	3.3	595
263	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	3.3	397
262	Electronic band structure, phonons, and exciton binding energies of halide perovskites CsSnCl3, CsSnBr3, and CsSnI3. *Physical Review B*, **2013**, 88,	3.3	312
261	Efficient ab initio method for the calculation of frequency-dependent second-order optical response in semiconductors. *Physical Review B*, **1998**, 57, 3905-3919	3.3	307
260	Electronic structure of rare-earth nitrides using the LSDA+U approach: Importance of allowing 4f orbitals to break the cubic crystal symmetry. *Physical Review B*, **2007**, 75,	3.3	270
259	Calculated elastic constants and deformation potentials of cubic SiC. *Physical Review B*, **1991**, 44, 3685-3694	3.3	257
258	Diamond nucleation by hydrogenation of the edges of graphitic precursors. *Nature*, **1993**, 364, 607-610	50.4	245
257	Valence-band ordering and magneto-optic exciton fine structure in ZnO. *Physical Review B*, **2002**, 65,	3.3	229
256	Second-harmonic generation of I-III-VI2 chalcopyrite semiconductors: Effects of chemical substitutions. *Physical Review B*, **2001**, 63,	3.3	212
255	Effective masses and valence-band splittings in GaN and AlN. *Physical Review B*, **1997**, 56, 7363-7375	3.3	204
254	Electronic and crystal structure of Cu2□S: Full-potential electronic structure calculations. *Physical Review B*, **2007**, 76,	3.3	202
253	Valence-band discontinuity between GaN and AlN measured by x-ray photoemission spectroscopy. *Applied Physics Letters*, **1994**, 65, 610-612	3.4	187
252	Electronic structure of GaN with strain and phonon distortions. *Physical Review B*, **1994**, 50, 1502-1505	3.3	179
251	Theoretical study of the relative stability of wurtzite and rocksalt phases in MgO and GaN. *Physical Review B*, **2001**, 63,	3.3	152
250	Stacking fault band structure in 4H□SiC and its impact on electronic devices. *Applied Physics Letters*, **2001**, 79, 4360-4362	3.4	149
249	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	3.3	148

248	High field electron transport properties of bulk ZnO. *Journal of Applied Physics*, **1999**, 86, 6864-6867	2.5	138
247	Homogeneous Strain Deformation Path for the Wurtzite to Rocksalt High-Pressure Phase Transition in GaN. *Physical Review Letters*, **2001**, 86, 91-94	7.4	131
246	First-principles calculation of the O vacancy in ZnO: A self-consistent gap-corrected approach. *Physical Review B*, **2008**, 77,	3.3	123
245	Self-consistent dipole theory of heterojunction band offsets. *Physical Review B*, **1990**, 41, 2813-2831	3.3	122
244	Electronic structure of rare-earth pnictides. *Physical Review B*, **1996**, 53, 4324-4339	3.3	110
243	Quasiparticle band structure of Zn-IV-N2 compounds. *Physical Review B*, **2011**, 84,	3.3	109
242	Electronic structure and bonding at SiC/AlN and SiC/BP interfaces. *Physical Review B*, **1991**, 43, 7070-7085	3.3	108
241	Electronic structure and properties of NiSi2 and CoSi2 in the fluorite and adamantane structures. *Physical Review B*, **1987**, 36, 2493-2503	3.3	103
240	Electronic structure and equilibrium properties of GaxAl1-xN alloys. *Physical Review B*, **1993**, 48, 17841-17847	3.3	96
239	Rare-earth mononitrides. *Progress in Materials Science*, **2013**, 58, 1316-1360	42.2	93
238	X-ray photoelectron spectroscopy and theory of the valence band and semicore Ga 3d states in GaN. *Physical Review B*, **1994**, 50, 14155-14160	3.3	93
237	Total energy differences between SiC polytypes revisited. *Physical Review B*, **1998**, 57, 12017-12022	3.3	92
236	Anomalous band-gap behavior and phase stability of c-BN-diamond alloys. *Physical Review B*, **1993**, 47, 9289-9296	3.3	90
235	Electronic band structure trends of perovskite halides: Beyond Pb and Sn to Ge and Si. *Physical Review B*, **2016**, 93,	3.3	86
234	Second-harmonic generation and birefringence of some ternary pnictide semiconductors. *Physical Review B*, **1999**, 59, 2737-2748	3.3	80
233	Electronic band structure of ordered vacancy defect chalcopyrite compounds with formula II□I2▽I4. *Physical Review B*, **2004**, 69,	3.3	79
232	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,	3.3	78
231	Charge-neutral disorder and polytypes in heterovalent wurtzite-based ternary semiconductors: The importance of the octet rule. *Physical Review B*, **2015**, 91,	3.3	76

230	Band offsets between ZnGeN2, GaN, ZnO, and ZnSnN2 and their potential impact for solar cells. *Physical Review B*, **2013**, 88,	3.3	72
229	Tight-binding muffin-tin orbital Green function method for surface and interface electronic structure calculations. *Surface Science*, **1986**, 178, 256-263	1.8	72
228	Magnetic properties of substitutional 3d transition metal impurities in silicon carbide. *Physical Review B*, **2003**, 68,	3.3	71
227	Atomic-scale spin-polarized scanning tunneling microscopy applied to Mn3N2(010). *Physical Review Letters*, **2002**, 89, 226101	7.4	70
226	Electronic structure of (diamond C)/(sphalerite BN) (110) interfaces and superlattices. *Physical Review B*, **1989**, 40, 9909-9919	3.3	68
225	Ferromagnetic redshift of the optical gap in GdN. *Physical Review B*, **2007**, 76,	3.3	67
224	UV reflectivity of GaN: Theory and experiment. *Physical Review B*, **1995**, 51, 13516-13532	3.3	67
223	Single crystal V2O5 and lower oxides. A survey of their electronic, optical, structural, and surface properties. *Physica Status Solidi A*, **1980**, 59, 485-504		66
222	Application of generalized gradient-corrected density functionals to iron. *Physical Review B*, **1992**, 46, 1870-1873	3.3	65
221	Universal transition state for high-pressure zinc blende to rocksalt phase transitions. *Physical Review Letters*, **2005**, 94, 225501	7.4	64
220	Electronic structure of CrN: A borderline Mott insulator. *Physical Review B*, **2009**, 79,	3.3	62
219	First-principles calculations of elasticity, polarization-related properties, and nonlinear optical coefficients in Zn-IV-N2 compounds. *Physical Review B*, **2009**, 79,	3.3	61
218	First-principles study of phonons and related ground-state properties and spectra in Zn-IV-N2 compounds. *Physical Review B*, **2008**, 78,	3.3	61
217	Interface-bond-polarity model for semiconductor heterojunction band offsets. *Physical Review B*, **1990**, 41, 2832-2848	3.3	60
216	Interstitial-nitrogen- and oxygen-induced magnetism in Gd-doped GaN. *Physical Review B*, **2009**, 80,	3.3	59
215	Band structure parameters of wurtzite and zinc-blende GaAs under strain in the GW approximation. *Physical Review B*, **2011**, 84,	3.3	58
214	First-principles study of the preference for zinc-blende or rocksalt structures in FeN and CoN. *Physical Review B*, **2004**, 70,	3.3	56
213	Electronic structure and magnetic interactions in MnN and Mn3N2. *Physical Review B*, **2003**, 68,	3.3	55

212	Lattice dynamics in perovskite halides CsSnX3 with X=I, Br, Cl. *Physical Review B*, **2014**, 90,	3.3	54
211	Band-structure analysis of the conduction-band mass anisotropy in 6H and 4H SiC. *Physical Review B* , **1995**, 52, R2249-R2252	3.3	54
210	Valence band structure of polytypic zinc-blende/wurtzite GaAs nanowires probed by polarization-dependent photoluminescence. *Physical Review B*, **2012**, 85,	3.3	53
209	Electronic structure and magnetism in Bi2Te3, Bi2Se3, and Sb2Te3 doped with transition metals (Ti□n). *Physical Review B*, **2008**, 78,	3.3	53
208	Electronic structure of Gd pnictides calculated within the LSDA+U approach. *Physical Review B*, **2006**, 74,	3.3	52
207	Optical-absorption bands in the 1□ eV range in n-type SiC polytypes. *Physical Review B*, **1999**, 59, 12890-12899	3.3	51
206	Calculated and measured uv reflectivity of SiC polytypes. *Physical Review B*, **1994**, 50, 10722-10726	3.3	51
205	Theory of semiconductor heterojunction valence-band offsets: From supercell band-structure calculations toward a simple model. *Physical Review Letters*, **1988**, 61, 1764-1767	7.4	51
204	Electronic structure of wide-band-gap ternary pnictides with the chalcopyrite structure. *Physical Review B*, **1994**, 49, 4549-4558	3.3	50
203	Electronic driving force for stacking fault expansion in 4H-SiC. *Physical Review B*, **2006**, 73,	3.3	49
202	Unified path for high-pressure transitions of SiC polytypes to the rocksalt structure. *Physical Review B*, **2003**, 68,	3.3	49
201	Second-harmonic generation in SiC polytypes. *Physical Review B*, **1998**, 57, 9705-9715	3.3	46
200	Electronic and lattice dynamical properties of II-IV-N2 semiconductors. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2011**, 8, 2492-2499		45
199	Electronic structure and magnetic properties of transition-metal-doped 3C and 4H silicon carbide. *Physical Review B*, **2006**, 74,	3.3	45
198	Graphitization Effects on Diamond Surfaces and the Diamond/Graphite Interface. *Physica Status Solidi A*, **1996**, 154, 109-125		45
197	Electronic structure of dense amorphous carbon. *Physical Review B*, **1994**, 49, 11448-11451	3.3	43
196	Optical reflectivity of 3C and 4H-SiC polytypes: Theory and experiment. *Applied Physics Letters*, **1993**, 63, 2747-2749	3.4	42
195	The energy band structure of V2O5. I. Theoretical approach and band calculations. *Journal of Physics C: Solid State Physics*, **1980**, 13, 2485-2500		42

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193	Strain effects on the spin-orbit-induced band structure splittings in monolayer MoS2 and graphene. *Physical Review B*, **2013**, 88,	3.3	40
192	Comparison between experiment and calculated band structures for DyN and SmN. *Physical Review B*, **2007**, 76,	3.3	40
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190	Electronic band structure of MgIVN2 compounds in the quasiparticle-self-consistent GW approximation. *Physical Review B*, **2016**, 94,	3.3	39
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188	Electronic structure and magnetism of the semimetals ErAs and ErxSc1-xAs. *Physical Review B*, **1994** , 50, 7800-7804	3.3	39
187	Native point defects and doping in ZnGeN2. *Physical Review B*, **2016**, 93,	3.3	38
186	X-ray absorption, glancing-angle reflectivity, and theoretical study of the N K- and Ga M2,3-edge spectra in GaN. *Physical Review B*, **1997**, 55, 2612-2622	3.3	38
185	Stability and half-metallicity of transition metal pnictides in tetrahedrally bonded structures. *Physical Review B*, **2005**, 71,	3.3	37
184	Pressure dependence of sound velocities in 3CSiC and their relation to the high-pressure phase transition. *Physical Review B*, **2002**, 66,	3.3	37
183	Structure and phonons of ZnGeN2. *Physical Review B*, **2005**, 72,	3.3	36
182	Valence band effective-mass Hamiltonians for the group-III nitrides from quasiparticle self-consistent GW band structures. *Physical Review B*, **2012**, 85,	3.3	35
181	Which electronic structure method for the study of defects: A commentary. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 1547-1558	1.3	35
180	Magnetic exchange interactions in the gadolinium pnictides from first principles. *Physical Review B*, **2008**, 78,	3.3	35
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178	Vibrational modes in ZnGeN2: Raman study and theory. *Physical Review B*, **2008**, 77,	3.3	34
177	Proton irradiation induced defects in Ga2O3: A combined EPR and theory study. *APL Materials*, **2019**, 7, 022521	5.7	33

176	Quasiparticle self-consistent GW calculations of the electronic band structure of bulk and monolayer V2O5. *Physical Review B*, **2015**, 91,	3.3	33
175	First-principles study of the elasticity, piezoelectricity, and vibrational modes in LiGaO2 compared with ZnO and GaN. *Physical Review B*, **2010**, 81,	3.3	33
174	Heteroepitaxy of diamond on c-BN: Growth mechanisms and defect characterization. *Journal of Materials Research*, **1994**, 9, 1849-1865	2.5	33
173	Disorder effects on the band structure of ZnGeN2: Role of exchange defects. *Physical Review B*, **2016**, 94,	3.3	31
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168	On the origin of the split-off conduction bands in V2O5. *Journal of Physics C: Solid State Physics*, **1981**, 14, 4785-4795		30
167	Structure and magnetic properties of MnN, CrN, and VN under volume expansion. *Physical Review B* , **2005**, 71,	3.3	28
166	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,	3.3	28
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154	Electronic structure of BeCN2: A proposed nearly direct wide-band-gap semiconductor. *Physical Review B*, **1992**, 45, 1485-1487	3.3	24
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151	Quasiparticle self-consistent GW band structure of Ga2O3 and the anisotropy of the absorption onset. *Applied Physics Letters*, **2017**, 110, 132103	3.4	22
150	Computational identification of Ga-vacancy related electron paramagnetic resonance centers in Ga2O3. *Journal of Applied Physics*, **2019**, 125, 185701	2.5	22
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145	Vibrational properties of rare-earth nitrides: Raman spectra and theory. *Physical Review B*, **2009**, 79,	3.3	21
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141	All-electron quasiparticle self-consistent GW band structures for SrTiO3 including lattice polarization corrections in different phases. *Physical Review Materials*, **2018**, 2,	3.2	21

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136	Electronic structure of thin heterocrystalline superlattices in SiC and AlN. *Physical Review B*, **2003**, 68,	3.3	19
135	Strong enhancement of second-order response coefficients in tellurium containing AgIIVI2 compounds. *Applied Physics Letters*, **2000**, 77, 190-192	3.4	19
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132	Electronic structure of defects and doping in ZnO: Oxygen vacancy and nitrogen doping. *Physica Status Solidi (B): Basic Research*, **2013**, 250, n/a-n/a	1.3	18
131	Electronic band structure information of GdN extracted from x-ray absorption and emission spectroscopy. *Applied Physics Letters*, **2010**, 96, 032101	3.4	18
130	Spin-orbit effects on the band structure and Fermi surface of ErAs and ErxSc1AAs. *Physical Review B*, **1997**, 55, 9239-9242	3.3	18
129	Electronic structure and magnetic properties of Mn3GaN precipitates in Ga1MnxN. *Physical Review B*, **2005**, 72,	3.3	18
128	Investigation of the stability of the hexagonalcubic born nitride prism interface. *Journal of Materials Chemistry*, **1996**, 6, 899-901		18
127	Optoelectronic Dichotomy of Mixed Halide CHNHPb(BrCl) Single Crystals: Surface versus Bulk Photoluminescence. *Journal of the American Chemical Society*, **2018**, 140, 11811-11819	16.4	18
126	Electronic structure, Schottky barrier, and optical spectra of the SiC/TiC {111} interface. *Physical Review B*, **1997**, 55, 16472-16486	3.3	17
125	First-principles calculations of second-order optical response functions in chalcopyrite semiconductors. *Journal of Physics and Chemistry of Solids*, **2003**, 64, 1615-1619	3.9	17
124	Theoretical evaluation of LiGaO_2 for frequency upconversion to ultraviolet. *Journal of the Optical Society of America B: Optical Physics*, **1999**, 16, 2217	1.7	17
123	XPS Measurement of the SiC/AlN Band-Offset at the (0001) Interface. *Materials Research Society Symposia Proceedings*, **1995**, 395, 375		17

122	Band Gaps, Band-Offsets, Disorder, Stability Region, and Point Defects in II-IV-N2 Semiconductors. *Physica Status Solidi (A) Applications and Materials Science*, **2019**, 216, 1800875	1.6	16
121	Electronic structure of defects and doping in ZnO: Oxygen vacancy and nitrogen doping. *Physica Status Solidi (B): Basic Research*, **2013**, 250, 2091-2101	1.3	16
120	Effects of structural relaxation, interdiffusion, and surface termination on two-dimensional electron gas formation at the LaAlO3/SrTiO3 (001) interface. *Physical Review B*, **2015**, 92,	3.3	16
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113	Schottky barrier formation at ErAs/GaAs interfaces: a case of Fermi level pinning by surface states. *Solid State Communications*, **1998**, 108, 361-365	1.6	14
112	Crystal structure, electronic structure and magnetism of transition metal nitrides. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2005**, 2, 2516-2519		14
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107	Carrier-controlled anomalous Hall effect in an intrinsic ferromagnetic semiconductor. *Physical Review B*, **2017**, 96,	3.3	12
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100	Vibrational spectra and nonlinear optical coefficients of rhombohedral CsGeX3 halide compounds with X=I, Br, Cl. *Physical Review B*, **2016**, 94,	3.3	11
99	Molecular-dynamics study of diamond/silicon (001) interfaces with and without graphitic interface layers. *Physical Review B*, **1997**, 56, 1568-1580	3.3	11
98	Electronic Structure and Optical Properties of ZnGeN2. *MRS Internet Journal of Nitride Semiconductor Research*, **1999**, 4, 600-605		11
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95	Electronic structure of the vanadyl oxygen vacancy in V2O5 : periodic vacancy single layer model. *Solid State Communications*, **1981**, 39, 257-261	1.6	11
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91	First-principles calculations of phonons and Raman spectra in monoclinic CsSnCl3. *Physical Review B* , **2015**, 91,	3.3	9
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89	Optical conductivity and x-ray absorption and emission study of the band structure of MnN films. *Physical Review B*, **2005**, 72,	3.3	9
88	Structural studies and electronic properties of diamond-like amorphous carbon. *Journal of Non-Crystalline Solids*, **1993**, 164-166, 1131-1134	3.9	9
87	Elastic Constants and Related Properties of the Group III-Nitrides. *Materials Research Society Symposia Proceedings*, **1995**, 395, 399		9

86	Electronic structure of SiCTiC interfaces. *Acta Metallurgica Et Materialia*, **1992**, 40, S17-S24		9
85	On the relation between XPS and AES relaxation energies in metals. *Journal of Electron Spectroscopy and Related Phenomena*, **1987**, 42, 161-169	1.7	9
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