Chris G. Van de Walle

List of Publications by Citations

528 papers	51,985 citations	108 h-index	219 g-index
554 ext. papers	56,685 ext. citations	4.3 avg, IF	8.22 L-index

#	Paper	IF	Citations
528	Fundamentals of zinc oxide as a semiconductor. *Reports on Progress in Physics*, **2009**, 72, 126501	14.4	2712
527	First-principles calculations for defects and impurities: Applications to III-nitrides. *Journal of Applied Physics*, **2004**, 95, 3851-3879	2.5	2330
526	Hydrogen as a cause of doping in zinc oxide. *Physical Review Letters*, **2000**, 85, 1012-5	7.4	1890
525	Native point defects in ZnO. *Physical Review B*, **2007**, 76,	3.3	1820
524	Band lineups and deformation potentials in the model-solid theory. *Physical Review B*, **1989**, 39, 1871-1883	3.3	1755
523	First-principles study of native point defects in ZnO. *Physical Review B*, **2000**, 61, 15019-15027	3.3	1454
522	First-principles calculations for point defects in solids. *Reviews of Modern Physics*, **2014**, 86, 253-305	40.5	1431
521	Theoretical calculations of heterojunction discontinuities in the Si/Ge system. *Physical Review B*, **1986**, 34, 5621-5634	3.3	1192
520	Universal alignment of hydrogen levels in semiconductors, insulators and solutions. *Nature*, **2003**, 423, 626-8	50.4	1003
519	Gallium vacancies and the yellow luminescence in GaN. *Applied Physics Letters*, **1996**, 69, 503-505	3.4	963
518	Oxygen vacancies in ZnO. *Applied Physics Letters*, **2005**, 87, 122102	3.4	887
517	Fully ab initio finite-size corrections for charged-defect supercell calculations. *Physical Review Letters*, **2009**, 102, 016402	7.4	845
516	Atomic geometry and electronic structure of native defects in GaN. *Physical Review B*, **1994**, 50, 8067-8070	3.3	692
515	Hydrogen multicentre bonds. *Nature Materials*, **2007**, 6, 44-7	27	600
514	Oxygen vacancies and donor impurities in □Ga2O3. *Applied Physics Letters*, **2010**, 97, 142106	3.4	581
513	Density-functional calculations for III-V nitrides using the local-density approximation and the generalized gradient approximation. *Physical Review B*, **1999**, 59, 5521-5535	3.3	564
512	Theoretical study of band offsets at semiconductor interfaces. *Physical Review B*, **1987**, 35, 8154-8165	3.3	533

511	Ultrawide-Bandgap Semiconductors: Research Opportunities and Challenges. *Advanced Electronic Materials*, **2018**, 4, 1600501	6.4	520
510	Hybrid functional studies of the oxygen vacancy in TiO2. *Physical Review B*, **2010**, 81,	3.3	486
509	Theory of hydrogen diffusion and reactions in crystalline silicon. *Physical Review B*, **1989**, 39, 10791-10808	3.3	458
508	Carbon impurities and the yellow luminescence in GaN. *Applied Physics Letters*, **2010**, 97, 152108	3.4	456
507	Quantum computing with defects. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 8513-8	11.5	453
506	Hydrogen in GaN: Novel aspects of a common impurity. *Physical Review Letters*, **1995**, 75, 4452-4455	7.4	390
505	Indirect Auger recombination as a cause of efficiency droop in nitride light-emitting diodes. *Applied Physics Letters*, **2011**, 98, 161107	3.4	388
504	Heterojunction band offset engineering. *Surface Science Reports*, **1996**, 25, 1-140	12.9	370
503	Effects of strain on band structure and effective masses in MoS2. *Physical Review B*, **2012**, 86,	3.3	353
502	Why nitrogen cannot lead to p-type conductivity in ZnO. *Applied Physics Letters*, **2009**, 95, 252105	3.4	339
501	Role of self-trapping in luminescence and p-type conductivity of wide-band-gap oxides. *Physical Review B*, **2012**, 85,	3.3	328
500	Hydrogen-related defects in ZnO studied by infrared absorption spectroscopy. *Physical Review B*, **2002**, 66,	3.3	311
499	Electrostatic interactions between charged defects in supercells. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 1067-1076	1.3	309
498	Sources of electrical conductivity in SnO2. *Physical Review Letters*, **2008**, 101, 055502	7.4	309
497	Effects of cation d states on the structural and electronic properties of III-nitride and II-oxide wide-band-gap semiconductors. *Physical Review B*, **2006**, 74,	3.3	301
496	Direct view at excess electrons in TiO2 rutile and anatase. *Physical Review Letters*, **2014**, 113, 086402	7.4	300
495	Auger recombination rates in nitrides from first principles. *Applied Physics Letters*, **2009**, 94, 191109	3.4	297
494	Effects of carbon on the electrical and optical properties of InN, GaN, and AlN. *Physical Review B*, **2014**, 89,	3.3	290

493	New insights into the role of native point defects in ZnO. *Journal of Crystal Growth*, **2006**, 287, 58-65	1.6	290
492	Band bowing and band alignment in InGaN alloys. *Applied Physics Letters*, **2010**, 96, 021908	3.4	288
491	Energies of various configurations of hydrogen in silicon. *Physical Review B*, **1994**, 49, 4579-4585	3.3	285
490	Role of hydrogen in doping of GaN. *Applied Physics Letters*, **1996**, 68, 1829-1831	3.4	278
489	Energetics and electronic structure of stacking faults in AlN, GaN, and InN. *Physical Review B*, **1998**, 57, R15052-R15055	3.3	273
488	First-principles calculations of solubilities and doping limits: Li, Na, and N in ZnSe. *Physical Review B*, **1993**, 47, 9425-9434	3.3	261
487	Native defects and self-compensation in ZnSe. *Physical Review B*, **1992**, 45, 10965-10978	3.3	253
486	Electronic structure and phase stability of GaAs1-xNx alloys. *Physical Review B*, **1995**, 51, 10568-10571	3.3	251
485	High-voltage field effect transistors with wide-bandgap Ga2O3 nanomembranes. *Applied Physics Letters*, **2014**, 104, 203111	3.4	242
484	Hybrid functional investigations of band gaps and band alignments for AlN, GaN, InN, and InGaN. *Journal of Chemical Physics*, **2011**, 134, 084703	3.9	228
483	Diffusivity of native defects in GaN. *Physical Review B*, **2004**, 69,	3.3	226
482	Theory of hydrogen diffusion and reactions in crystalline silicon. *Physical Review Letters*, **1988**, 60, 2761-2764	7.4	220
481	Defect analysis and engineering in ZnO. *Physica B: Condensed Matter*, **2001**, 308-310, 899-903	2.8	218
480	Microscopic origins of surface states on nitride surfacesa). *Journal of Applied Physics*, **2007**, 101, 081704	2.5	217
479	First-principles surface phase diagram for hydrogen on GaN surfaces. *Physical Review Letters*, **2002**, 88, 066103	7.4	216
478	Experimental electronic structure of In2O3and Ga2O3. *New Journal of Physics*, **2011**, 13, 085014	2.9	213
477	Effect of Si doping on strain, cracking, and microstructure in GaN thin films grown by metalorganic chemical vapor deposition. *Journal of Applied Physics*, **2000**, 87, 7745-7752	2.5	211
476	Interactions of hydrogen with native defects in GaN. *Physical Review B*, **1997**, 56, R10020-R10023	3.3	210

475	First-principles calculations of hyperfine parameters. *Physical Review B*, **1993**, 47, 4244-4255	3.3	208
474	Shallow versus deep nature of Mg acceptors in nitride semiconductors. *Physical Review Letters*, **2012**, 108, 156403	7.4	207
473	Tutorial: Defects in semiconductors□combining experiment and theory. *Journal of Applied Physics*, **2016**, 119, 181101	2.5	206
472	Defect formation energies without the band-gap problem: combining density-functional theory and the GW approach for the silicon self-interstitial. *Physical Review Letters*, **2009**, 102, 026402	7.4	196
471	Theoretical investigation of native defects, impurities, and complexes in aluminum nitride. *Physical Review B*, **2002**, 65,	3.3	196
470	Native defects and impurities in InN: First-principles studies using the local-density approximation and self-interaction and relaxation-corrected pseudopotentials. *Physical Review B*, **2000**, 61, R7846-R7849	3.3	196
469	Electrostatic carrier doping of GdTiO3/SrTiO3 interfaces. *Applied Physics Letters*, **2011**, 99, 232116	3.4	195
468	Optical characterization and band offsets in ZnSe-ZnSxSe. *Physical Review B*, **1988**, 38, 1417-1426	3.3	188
467	Large band gap bowing of InxGa1□N alloys. *Applied Physics Letters*, **1998**, 72, 2725-2726	3.4	187
466	Hydrogenated cation vacancies in semiconducting oxides. *Journal of Physics Condensed Matter*, **2011**, 23, 334212	1.8	186
465	Theoretical study of Si/Ge interfaces. *Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena*, **1985**, 3, 1256		177
464	Brillouin zone and band structure of □Ga2O3. *Physica Status Solidi (B): Basic Research*, **2015**, 252, 828-832	1.3	176
463	Theory of doping and defects in III□V nitrides. *Journal of Crystal Growth*, **1998**, 189-190, 505-510	1.6	175
462	Origins of Fermi-level pinning on GaN and InN polar and nonpolar surfaces. *Europhysics Letters*, **2006**, 76, 305-311	1.6	169
461	First-principles theory of nonradiative carrier capture via multiphonon emission. *Physical Review B*, **2014**, 90,	3.3	168
460	Native point defects and dangling bonds in □Al2O3. *Journal of Applied Physics*, **2013**, 113, 044501	2.5	165
459	Vacancies and small polarons in SrTiO3. *Physical Review B*, **2014**, 90,	3.3	156
458	Electronic properties of the (100) (Si)/(Ge) strained-layer superlattices. *Physical Review B*, **1988**, 38, 13237-13245	3.3	155

457	"Absolute" deformation potentials: Formulation and ab initio calculations for semiconductors. *Physical Review Letters*, **1989**, 62, 2028-2031	7.4	152
456	Theoretical calculations of semiconductor heterojunction discontinuities. *Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena*, **1986**, 4, 1055		152
455	Energy levels of isolated interstitial hydrogen in silicon. *Physical Review B*, **2001**, 64,	3.3	151
454	Indium incorporation and emission properties of nonpolar and semipolar InGaN quantum wells. *Applied Physics Letters*, **2012**, 100, 201108	3.4	148
453	Hydrogen doping in indium oxide: An ab initio study. *Physical Review B*, **2009**, 80,	3.3	148
452	Mechanism of visible-light photocatalysis in nitrogen-doped TiO*Advanced Materials*, **2011**, 23, 2343-7	24	146
451	Microscopic structure of the hydrogen-boron complex in crystalline silicon. *Physical Review B*, **1989**, 39, 10809-10824	3.3	142
450	Computationally predicted energies and properties of defects in GaN. *Npj Computational Materials*, **2017**, 3,	10.9	141
449	Oxide interfaces for novel electronic applications. *New Journal of Physics*, **2014**, 16, 025005	2.9	141
448	Metastability of Oxygen Donors in AlGaN. *Physical Review Letters*, **1998**, 80, 4008-4011	7.4	138
447	Interplay of polarization fields and Auger recombination in the efficiency droop of nitride light-emitting diodes. *Applied Physics Letters*, **2012**, 101, 231107	3.4	137
446	Mechanisms of dopant impurity diffusion in silicon. *Physical Review B*, **1989**, 40, 5484-5496	3.3	137
445	Native defects in Al2O3 and their impact on III-V/Al2O3 metal-oxide-semiconductor-based devices. *Journal of Applied Physics*, **2011**, 109, 033715	2.5	135
444	Origin and passivation of fixed charge in atomic layer deposited aluminum oxide gate insulators on chemically treated InGaAs substrates. *Applied Physics Letters*, **2010**, 96, 152908	3.4	134
443	Hydrogen passivation effect in nitrogen-doped ZnO thin films. *Applied Physics Letters*, **2005**, 86, 122107	3.4	134
442	Strain effects in group-III nitrides: Deformation potentials for AlN, GaN, and InN. *Applied Physics Letters*, **2009**, 95, 121111	3.4	132
441	Native point defects and impurities in hexagonal boron nitride. *Physical Review B*, **2018**, 97,	3.3	131
440	First-principles optical spectra for F centers in MgO. *Physical Review Letters*, **2012**, 108, 126404	7.4	131

439	First-principles calculations of luminescence spectrum line shapes for defects in semiconductors: the example of GaN and ZnO. *Physical Review Letters*, **2012**, 109, 267401	7.4	131
438	DX-center formation in wurtzite and zinc-blende AlxGa1□N. *Physical Review B*, **1998**, 57, R2033-R2036	3.3	131
437	Tin dioxide from first principles: Quasiparticle electronic states and optical properties. *Physical Review B*, **2011**, 83,	3.3	129
436	Doping of AlxGa1□N. *Applied Physics Letters*, **1998**, 72, 459-461	3.4	129
435	Structural and electronic properties of Ga2O3-Al2O3 alloys. *Applied Physics Letters*, **2018**, 112, 242101	3.4	127
434	The electronic structure of □Ga2O3. *Applied Physics Letters*, **2010**, 97, 211903	3.4	127
433	HYDROGEN IN SEMICONDUCTORS. *Annual Review of Materials Research*, **2006**, 36, 179-198	12.8	127
432	Dual behavior of excess electrons in rutile TiO2. *Physica Status Solidi - Rapid Research Letters*, **2013**, 7, 199-203	2.5	126
431	Polarization-driven topological insulator transition in a GaN/InN/GaN quantum well. *Physical Review Letters*, **2012**, 109, 186803	7.4	124
430	First-principles studies of beryllium doping of GaN. *Physical Review B*, **2001**, 63,	3.3	124
429	Small valence-band offsets at GaN/InGaN heterojunctions. *Applied Physics Letters*, **1997**, 70, 2577-2579	3.4	122
428	First-principles theory of the luminescence lineshape for the triplet transition in diamond NV centres. *New Journal of Physics*, **2014**, 16, 073026	2.9	121
427	Absolute deformation potentials and band alignment of wurtzite ZnO, MgO, and CdO. *Physical Review B*, **2007**, 75,	3.3	121
426	Role of native defects in wide-band-gap semiconductors. *Physical Review Letters*, **1991**, 66, 648-651	7.4	120
425	Measurement and Control of Single Nitrogen-Vacancy Center Spins above 600 K. *Physical Review X*, **2012**, 2,	9.1	117
424	Exciton-dominated Dielectric Function of Atomically Thin MoS2 Films. *Scientific Reports*, **2015**, 5, 16996	4.9	114
423	Nature and evolution of the band-edge states in MoS2: From monolayer to bulk. *Physical Review B*, **2014**, 90,	3.3	110
422	Phonon-assisted optical absorption in silicon from first principles. *Physical Review Letters*, **2012**, 108, 167402	7.4	110

421	Dangling-bond defects and hydrogen passivation in germanium. *Applied Physics Letters*, **2007**, 91, 142101	3.4	110
420	Role of nitrogen vacancies in the luminescence of Mg-doped GaN. *Applied Physics Letters*, **2012**, 100, 142110	3.4	107
419	Structure and properties of hydrogen-impurity pairs in elemental semiconductors. *Physical Review Letters*, **1989**, 62, 1884-1887	7.4	103
418	Quantitative analysis of the polarization fields and absorption changes in InGaN/GaN quantum wells with electroabsorption spectroscopy. *Applied Physics Letters*, **2002**, 81, 490-492	3.4	102
417	LDA + U and hybrid functional calculations for defects in ZnO, SnO2, and TiO2. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 799-804	1.3	100
416	Energetics and Vibrational Frequencies of Interstitial H2 Molecules in Semiconductors. *Physical Review Letters*, **1998**, 80, 2177-2180	7.4	100
415	Hybrid functional calculations of DX centers in AlN and GaN. *Physical Review B*, **2014**, 89,	3.3	97
414	Free-carrier absorption in nitrides from first principles. *Physical Review B*, **2010**, 81,	3.3	97
413	Inverted order of acceptor and donor levels of monatomic hydrogen in silicon. *Physical Review Letters*, **1994**, 73, 130-133	7.4	97
412	Fluorine-silicon reactions and the etching of crystalline silicon. *Physical Review Letters*, **1988**, 61, 1867-1870	7.4	96
411	Origins of optical absorption and emission lines in AlN. *Applied Physics Letters*, **2014**, 105, 111104	3.4	94
410	Clean and As-Covered Zinc-Blende GaN (001) Surfaces: Novel Surface Structures and Surfactant Behavior. *Physical Review Letters*, **1998**, 80, 3097-3100	7.4	92
409	First-principles theory of acceptors in nitride semiconductors. *Physica Status Solidi (B): Basic Research*, **2015**, 252, 900-908	1.3	90
408	Effects of doping on the lattice parameter of SrTiO3. *Applied Physics Letters*, **2012**, 100, 262104	3.4	90
407	First-principles investigation of visible light emission from silicon-based materials. *Physical Review Letters*, **1993**, 70, 1116-1119	7.4	88
406	Mechanisms of equilibrium and nonequilibrium diffusion of dopants in silicon. *Physical Review Letters*, **1989**, 62, 1049-1052	7.4	88
405	Effects of hydrogen on the electronic properties of dilute GaAsN alloys. *Physical Review Letters*, **2002**, 89, 086403	7.4	87
404	Interactions between hydrogen impurities and vacancies in Mg and Al: A comparative analysis based on density functional theory. *Physical Review B*, **2009**, 80,	3.3	86

403	Acceptor doping in ZnSe versus ZnTe. *Applied Physics Letters*, **1993**, 63, 1375-1377	3.4	86
402	Temperature and carrier-density dependence of Auger and radiative recombination in nitride optoelectronic devices. *New Journal of Physics*, **2013**, 15, 125006	2.9	85
401	Role of charged defects and impurities in kinetics of hydrogen storage materials: A first-principles study. *Physical Review B*, **2007**, 76,	3.3	85
400	Deep acceptors and their diffusion in Ga2O3. *APL Materials*, **2019**, 7, 022519	5.7	84
399	Impact of carbon and nitrogen impurities in high-□dielectrics on metal-oxide-semiconductor devices. *Applied Physics Letters*, **2013**, 102, 142902	3.4	84
398	Strategies for Controlling the Conductivity of Wide-Band-Gap Semiconductors. *Physica Status Solidi (B): Basic Research*, **2002**, 229, 221-228	1.3	84
397	Chemical trends for acceptor impurities in GaN. *Journal of Applied Physics*, **1999**, 85, 3003-3005	2.5	84
396	Surface reconstructions on InN and GaN polar and nonpolar surfaces. *Surface Science*, **2007**, 601, L15-L18	1.8	83
395	Interactions between nitrogen, hydrogen, and gallium vacancies in GaAs1□Nx alloys. *Physical Review B*, **2003**, 67,	3.3	83
394	Shallow donor state of hydrogen in indium nitride. *Applied Physics Letters*, **2003**, 82, 592-594	3.4	83
393	Comment on □eduction of hot electron degradation in metal oxide semiconductor transistors by deuterium processing□[Appl. Phys. Lett. 68, 2526 (1996)]. *Applied Physics Letters*, **1996**, 69, 2441-2441	3.4	83
392	Fundamental limits on the electron mobility of □GaO. *Journal of Physics Condensed Matter*, **2017**, 29, 234001	1.8	81
391	Oxidation and the origin of the two-dimensional electron gas in AlGaN/GaN heterostructures. *Journal of Applied Physics*, **2010**, 107, 123713	2.5	81
390	Controlling the density of the two-dimensional electron gas at the SrTiO3/LaAlO3 interface. *Physical Review B*, **2012**, 86,	3.3	81
389	Causes of incorrect carrier-type identification in van der Pauw□all measurements. *Applied Physics Letters*, **2008**, 93, 242108	3.4	81
388	Microscopic structure of the hydrogen-phosphorus complex in crystalline silicon. *Physical Review B*, **1990**, 41, 3885-3888	3.3	81
387	Ambipolar doping in SnO. *Applied Physics Letters*, **2013**, 103, 082118	3.4	80
386	Sources of unintentional conductivity in InN. *Applied Physics Letters*, **2008**, 92, 032104	3.4	80

385	Fundamental limits on optical transparency of transparent conducting oxides: Free-carrier absorption in SnO2. *Applied Physics Letters*, **2012**, 100, 011914	3.4	78
384	Reconstructions and origin of surface states on AlN polar and nonpolar surfaces. *Physical Review B*, **2009**, 80,	3.3	78
383	First-principles calculations of diffusion coefficients: Hydrogen in silicon. *Physical Review Letters*, **1990**, 64, 1401-1404	7.4	78
382	Role of Si and Ge as impurities in ZnO. *Physical Review B*, **2009**, 80,	3.3	77
381	Absolute surface energies of polar and nonpolar planes of GaN. *Physical Review B*, **2014**, 89,	3.3	76
380	Tuning bad metal and non-Fermi liquid behavior in a Mott material: Rare-earth nickelate thin films. *Science Advances*, **2015**, 1, e1500797	14.3	76
379	The role of oxygen-related defects and hydrogen impurities in HfO2 and ZrO2. *Microelectronic Engineering*, **2011**, 88, 1452-1456	2.5	76
378	Magnesium incorporation in GaN grown by molecular-beam epitaxy. *Applied Physics Letters*, **2001**, 78, 285-287	3.4	76
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376	Effects of strain on the band structure of group-III nitrides. *Physical Review B*, **2014**, 90,	3.3	73
375	Strain effects on the electronic structure of SrTiO3: Toward high electron mobilities. *Physical Review B*, **2011**, 84,	3.3	72
374	Atomic arrangement at the AlN/SiC interface. *Physical Review B*, **1996**, 53, 7473-7478	3.3	72
373	Gallium vacancy complexes as a cause of Shockley-Read-Hall recombination in III-nitride light emitters. *Applied Physics Letters*, **2016**, 108, 141101	3.4	72
372	Effects of an Electrically Conducting Layer at the Zinc Oxide Surface. *Japanese Journal of Applied Physics*, **2005**, 44, 7271-7274	1.4	69
371	(InxGa1⁢)2O3 alloys for transparent electronics. *Physical Review B*, **2015**, 92,	3.3	68
370	First-principles characterization of native-defect-related optical transitions in ZnO. *Journal of Applied Physics*, **2017**, 122, 035704	2.5	67
369	Defects as qubits in 3C⁢and 4H⁢SiC. *Physical Review B*, **2015**, 92,	3.3	67
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365	Distribution of donor states on etched surface of AlGaN/GaN heterostructures. *Journal of Applied Physics*, **2010**, 108, 063719	2.5	66
364	Controlling the conductivity of InN. *Physica Status Solidi (A) Applications and Materials Science*, **2010**, 207, 1024-1036	1.6	66
363	Influence of microstructure on the carrier concentration of Mg-doped GaN films. *Applied Physics Letters*, **2001**, 79, 2734-2736	3.4	66
362	Role of oxygen vacancies in crystalline WO3. *Journal of Materials Chemistry C*, **2016**, 4, 6641-6648	7.1	65
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360	Role of excited states in Shockley-Read-Hall recombination in wide-band-gap semiconductors. *Physical Review B*, **2016**, 93,	3.3	61
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358	Self-consistent band-gap corrections in density functional theory using modified pseudopotentials. *Physical Review B*, **2007**, 75,	3.3	60
357	Silicon-hydrogen bonding and hydrogen diffusion in amorphous silicon. *Physical Review B*, **1995**, 51, 10615-10618	3.3	60
356	Theory of Point Defects and Complexes in GaN. *Materials Research Society Symposia Proceedings*, **1995**, 395, 645		60
355	Structural identification of hydrogen and muonium centers in silicon: First-principles calculations of hyperfine parameters. *Physical Review Letters*, **1990**, 64, 669-672	7.4	60
354	First-principles analysis of electron transport in BaSnO3. *Physical Review B*, **2017**, 95,	3.3	59
353	Structural origins of the properties of rare earth nickelate superlattices. *Physical Review B*, **2013**, 87,	3.3	59
352	Hydrogen interactions with acceptor impurities in SnO2: First-principles calculations. *Physical Review B*, **2009**, 79,	3.3	59
351	Analysis of a conducting channel at the native zinc oxide surface. *Superlattices and Microstructures*, **2006**, 39, 8-16	2.8	59
350	First-Principles Calculations of Point Defects for Quantum Technologies. *Annual Review of Materials Research*, **2018**, 48, 1-26	12.8	58

349	Polycrystalline nitride semiconductor light-emitting diodes fabricated on quartz substrates. *Applied Physics Letters*, **2000**, 76, 2182-2184	3.4	58
348	First-principles calculations of indirect Auger recombination in nitride semiconductors. *Physical Review B*, **2015**, 92,	3.3	57
347	Indium versus hydrogen-terminated GaN(0001) surfaces: Surfactant effect of indium in a chemical vapor deposition environment. *Applied Physics Letters*, **2004**, 84, 4322-4324	3.4	57
346	Strain effects and band parameters in MgO, ZnO, and CdO. *Applied Physics Letters*, **2012**, 101, 152105	3.4	56
345	Distributed surface donor states and the two-dimensional electron gas at AlGaN/GaN heterojunctions. *Journal Physics D: Applied Physics*, **2010**, 43, 505501	3	56
344	Determination of Internal Loss in Nitride Lasers from First Principles. *Applied Physics Express*, **2010**, 3, 082101	2.4	56
343	Monolayer to Bulk Properties of Hexagonal Boron Nitride. *Journal of Physical Chemistry C*, **2018**, 122, 25524-25529	3.8	56
342	Defects in SiC for quantum computing. *Journal of Applied Physics*, **2011**, 109, 102417	2.5	55
341	Large and composition-dependent band gap bowing in InxGa1⊠N alloys. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **1999**, 59, 274-278	3.1	55
340	Effect of composition on the band gap of strained InxGa1⊠N alloys. *Journal of Applied Physics*, **2003**, 93, 4340-4342	2.5	54
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337	Identification of hydrogen configurations in p-type GaN through first-principles calculations of vibrational frequencies. *Physical Review B*, **2003**, 68,	3.3	53
336	Effects of hole localization on limiting p-type conductivity in oxide and nitride semiconductors. *Journal of Applied Physics*, **2014**, 115, 012014	2.5	52
335	Electronic structure of nitride surfaces. *Journal of Crystal Growth*, **2007**, 300, 199-203	1.6	52
334	Arsenic impurities in GaN. *Applied Physics Letters*, **2000**, 76, 1009-1011	3.4	52
333	First-Principles Analysis of Radiative Recombination in Lead-Halide Perovskites. *ACS Energy Letters*, **2018**, 3, 2329-2334	20.1	52
332	First-principles study of the formation and migration of native defects in NaAlH4. *Physical Review B*, **2009**, 80,	3.3	50

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