Chris G. Van de Walle

List of Publications by Year in Descending Order

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	Defect tolerance in halide perovskites: A first-principles perspective. *Journal of Applied Physics*, **2022**, 131, 090901	2.5	4
527	Role of carbon and hydrogen in limiting n -type doping of monoclinic (AlxGa1□)2. *Physical Review B* , **2022**, 105,	3.3	3
526	Epitaxial ScxAl1□N on GaN exhibits attractive high-K dielectric properties. *Applied Physics Letters*, **2022**, 120, 152901	3.4	5
525	Incorporation of Si and Sn donors in □Ga2O3 through surface reconstructions. *Journal of Applied Physics*, **2021**, 130, 185703	2.5	3
524	All-inorganic halide perovskites as candidates for efficient solar cells. *Cell Reports Physical Science*, **2021**, 2, 100604	6.1	7
523	Prospects for n-type conductivity in cubic boron nitride. *Applied Physics Letters*, **2021**, 119, 162105	3.4	3
522	Surprising stability of polar (001) surfaces of the Mott insulator GdTiO3. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **2021**, 39, 063220	2.9	1
521	Thermodynamics of boron incorporation in BGaN. *Physical Review Materials*, **2021**, 5,	3.2	3
520	Finite-size correction for slab supercell calculations of materials with spontaneous polarization. *Npj Computational Materials*, **2021**, 7,	10.9	2
519	Minimizing hydrogen vacancies to enable highly efficient hybrid perovskites. *Nature Materials*, **2021** , 20, 971-976	27	33
518	Atomic scale investigation of aluminum incorporation, defects, and phase stability in □(AlxGa1□)2O3 films. *APL Materials*, **2021**, 9, 051103	5.7	20
517	Hydride Conductivity in Nitride Hydrides. *ACS Applied Energy Materials*, **2021**, 4, 6348-6355	6.1	2
516	Vibrational and vibronic structure of isolated point defects: The nitrogen-vacancy center in diamond. *Physical Review B*, **2021**, 104,	3.3	7
515	Defect Chemistry and Hydrogen Transport in La/Sr-Based Oxyhydrides. *Journal of Physical Chemistry C*, **2021**, 125, 2250-2256	3.8	1
514	Understanding carbon contamination in the proton-conducting zirconates and cerates. *Physical Chemistry Chemical Physics*, **2021**, 23, 14205-14211	3.6	0
513	Impact of dangling bonds on properties of h-BN. *2D Materials*, **2021**, 8, 024002	5.9	1
512	Boron dangling bonds in a monolayer of hexagonal boron nitride. *Journal of Applied Physics*, **2021**, 129, 064301	2.5	2

511	Adsorption and Diffusion of Aluminum on β-Ga2O(010) Surfaces. *ACS Applied Materials & Interfaces*, **2021**, 13, 10650-10655	9.5	5
510	A first-principles understanding of point defects and impurities in GaN. *Journal of Applied Physics*, **2021**, 129, 111101	2.5	19
509	Materials and device simulations for silicon qubit design and optimization. *MRS Bulletin*, **2021**, 46, 634-641	3.2	2
508	Hole Trapping at Acceptor Impurities and Alloying Elements in AlN. *Physica Status Solidi - Rapid Research Letters*, **2021**, 15, 2100218	2.5	2
507	First-principles study of electron transport in ScN. *Physical Review B*, **2021**, 104,	3.3	1
506	Piezoelectric effect and polarization switching in Al1-xScxN. *Journal of Applied Physics*, **2021**, 130, 104101	2.5	3
505	Structural, electronic, and polarization properties of YN and LaN. *Physical Review Materials*, **2021**, 5,	3.2	1
504	Nonrad: Computing nonradiative capture coefficients from first principles. *Computer Physics Communications*, **2021**, 267, 108056	4.2	12
503	Mg doping and diffusion in (010) β-Ga2O3 films grown by plasma-assisted molecular beam epitaxy. *Journal of Applied Physics*, **2021**, 130, 235301	2.5	2
502	Polarization properties at rocksalt/wurtzite oxide interfaces. *Physical Review B*, **2020**, 102,	3.3	2
501	Band alignments and polarization properties of the Zn-IV-nitrides. *Journal of Materials Chemistry C*, **2020**, 8, 7890-7898	7.1	12
500	Hidden role of Bi incorporation in nonradiative recombination in methylammonium lead iodide. *Journal of Materials Chemistry A*, **2020**, 8, 12964-12967	13	12
499	Prospects for high carrier mobility in the cubic germanates. *Semiconductor Science and Technology*, **2020**, 35, 085030	1.8	0
498	Role of Ga and In adatoms in the epitaxial growth of β-Ga2O3. *Physical Review B*, **2020**, 102,	3.3	6
497	First-principles study of transport in WO3. *Physical Review B*, **2020**, 101,	3.3	1
496	Correctly Assessing Defect Tolerance in Halide Perovskites. *Journal of Physical Chemistry C*, **2020**, 124, 6022-6027	3.8	35
495	Effect of Titanium Induced Chemical Inhomogeneity on Crystal Structure, Electronic Structure, and Optical Properties of Wide Band Gap Ga2O3. *Crystal Growth and Design*, **2020**, 20, 1422-1433	3.5	12
494	Spinning up quantum defects in 2D materials. *Nature Materials*, **2020**, 19, 487-489	27	9

493	Iodine interstitials as a cause of nonradiative recombination in hybrid perovskites. *Physical Review B* , **2020**, 101,	3.3	39
492	First-Principles Calculations 1. *Springer Series in Materials Science*, **2020**, 309-328	0.9	
491	Deep-Level Defects and Impurities in InGaN Alloys. *Physica Status Solidi (B): Basic Research*, **2020**, 257, 1900534	1.3	7
490	First-Principles Simulation of Carrier Recombination Mechanisms in Halide Perovskites. *Advanced Energy Materials*, **2020**, 10, 1902830	21.8	31
489	Anomalous Auger Recombination in PbSe. *Physical Review Letters*, **2020**, 125, 037401	7.4	6
488	First-principles calculations of hyperfine interaction, binding energy, and quadrupole coupling for shallow donors in silicon. *Npj Computational Materials*, **2020**, 6,	10.9	9
487	Electronic structure and magneto-optical properties of silicon-nitrogen-vacancy complexes in diamond. *Physical Review B*, **2020**, 102,	3.3	4
486	First-principles surface energies for monoclinic Ga2O3 and Al2O3 and consequences for cracking of (AlxGa1⊠)2O3. *APL Materials*, **2020**, 8, 091105	5.7	26
485	Radiative capture rates at deep defects from electronic structure calculations. *Physical Review B*, **2020**, 102,	3.3	7
484	Inflection points in the conduction-band structure of BaSnO3. *Physical Review B*, **2020**, 102,	3.3	2
483	Orientation-dependent band offsets between (AlxGa1⊠)2O3 and Ga2O3. *Applied Physics Letters*, **2020**, 117, 252104	3.4	14
482	First-principles study of electron-phonon interactions and transport in anatase TiO2. *Physical Review B*, **2019**, 100,	3.3	4
481	Deep acceptors and their diffusion in Ga2O3. *APL Materials*, **2019**, 7, 022519	5.7	84
480	First-principles study of bandgap bowing in BGaN alloys. *Journal of Applied Physics*, **2019**, 126, 095706	2.5	11
479	Limitations of In2O3 as a transparent conducting oxide. *Applied Physics Letters*, **2019**, 115, 082105	3.4	12
478	Dangling Bonds in Hexagonal Boron Nitride as Single-Photon Emitters. *Physical Review Letters*, **2019**, 123, 127401	7.4	38
477	Strategies for p-type doping of ZnGeN2. *Applied Physics Letters*, **2019**, 114, 032101	3.4	9
476	Hydrogen-Induced Degradation of NaMnO2. *Chemistry of Materials*, **2019**, 31, 5224-5228	9.6	5

475	Electrical and optical properties of iron in GaN, AlN, and InN. *Physical Review B*, **2019**, 99,	3.3	17
474	Optimizing Proton Conductivity in Zirconates through Defect Engineering. *ACS Applied Energy Materials*, **2019**, 2, 2611-2619	6.1	11
473	Phonon- and charged-impurity-assisted indirect free-carrier absorption in Ga2O3. *Physical Review B*, **2019**, 100,	3.3	7
472	Optimizing n-type doping of ZnGeN2 and ZnSiN2. *Physical Review B*, **2019**, 100,	3.3	4
471	Unusual Formation of Point-Defect Complexes in the Ultrawide-Band-Gap Semiconductor Ga2O3. *Physical Review X*, **2019**, 9,	9.1	43
470	Role of point defects in the electrical and optical properties of In2O3. *Physical Review Materials*, **2019**, 3,	3.2	21
469	First-principles study of antisite defects in perovskite stannates. *Journal of Applied Physics*, **2019**, 126, 195701	2.5	5
468	Carbon dimer defect as a source of the 4.1 eV luminescence in hexagonal boron nitride. *Applied Physics Letters*, **2019**, 115, 212101	3.4	37
467	Ab initio study of enhanced thermal conductivity in ordered AlGaO3 alloys. *Applied Physics Letters*, **2019**, 115, 242103	3.4	15
466	Giant polarization charge density at lattice-matched GaN/ScN interfaces. *Applied Physics Letters*, **2019**, 115, 232103	3.4	7
465	Comment on Comparative study of ab initio nonradiative recombination rate calculations under different formalisms *Physical Review B*, **2018**, 97,	3.3	8
464	Origins of n-type doping difficulties in perovskite stannates. *Physical Review B*, **2018**, 97,	3.3	30
463	First-Principles Calculations of Point Defects for Quantum Technologies. *Annual Review of Materials Research*, **2018**, 48, 1-26	12.8	58
462	Interfacial Cation-Defect Charge Dipoles in Stacked TiO/AlO Gate Dielectrics. *ACS Applied Materials & Interfaces*, **2018**, 10, 5140-5146	9.5	8
461	First-principles study of direct and indirect optical absorption in BaSnO3. *Applied Physics Letters*, **2018**, 112, 062106	3.4	11
460	Posner molecules: from atomic structure to nuclear spins. *Physical Chemistry Chemical Physics*, **2018**, 20, 12373-12380	3.6	19
459	Linear Hyperfine Tuning of Donor Spins in Silicon Using Hydrostatic Strain. *Physical Review Letters*, **2018**, 120, 167701	7.4	25
458	Accurate and efficient band-offset calculations from density functional theory. *Computational Materials Science*, **2018**, 151, 174-180	3.2	33

457	Ion-Transport Engineering of Alkaline-Earth Hydrides for Hydride Electrolyte Applications. *Chemistry of Materials*, **2018**, 30, 5878-5885	9.6	11
456	Electron doping in Sr3Ir2O7: Collapse of band gap and magnetic order. *Physical Review B*, **2018**, 98,	3.3	1
455	Native point defects and impurities in hexagonal boron nitride. *Physical Review B*, **2018**, 97,	3.3	131
454	Structural and electronic properties of Ga2O3-Al2O3 alloys. *Applied Physics Letters*, **2018**, 112, 242101	3.4	127
453	First-principles calculations of optical transitions at native defects and impurities in ZnO **2018**,		1
452	Impact of point defects on electrochromism in WO3 **2018**,		1
451	Ultrawide-Bandgap Semiconductors: Research Opportunities and Challenges. *Advanced Electronic Materials*, **2018**, 4, 1600501	6.4	520
450	Defect identification based on first-principles calculations for deep level transient spectroscopy. *Applied Physics Letters*, **2018**, 113, 192106	3.4	33
449	Monolayer to Bulk Properties of Hexagonal Boron Nitride. *Journal of Physical Chemistry C*, **2018**, 122, 25524-25529	3.8	56
448	Sr3Ir2O7F2: Topochemical conversion of a relativistic Mott state into a spin-orbit driven band insulator. *Physical Review B*, **2018**, 98,	3.3	2
447	First-Principles Analysis of Radiative Recombination in Lead-Halide Perovskites. *ACS Energy Letters*, **2018**, 3, 2329-2334	20.1	52
446	Unexpectedly Strong Auger Recombination in Halide Perovskites. *Advanced Energy Materials*, **2018**, 8, 1801027	21.8	36
445	Three-Dimensional Spin Texture in Hybrid Perovskites and Its Impact on Optical Transitions. *Journal of Physical Chemistry Letters*, **2018**, 9, 2903-2908	6.4	33
444	Carrier-induced absorption as a mechanism for electrochromism in tungsten trioxide. *MRS Communications*, **2018**, 8, 926-931	2.7	5
443	Calcium as a nonradiative recombination center in InGaN. *Applied Physics Express*, **2017**, 10, 021001	2.4	10
442	Ab initio study of hydrogenic effective mass impurities in Si nanowires. *Journal of Physics Condensed Matter*, **2017**, 29, 095303	1.8	1
441	Controlling n-Type Doping in MoO3. *Chemistry of Materials*, **2017**, 29, 2563-2567	9.6	49
440	Acceptor doping in the proton conductor SrZrO. *Physical Chemistry Chemical Physics*, **2017**, 19, 11485-11491	3.91	13

439	Identification of yellow luminescence centers in Be-doped GaN through pressure-dependent studies. *Journal Physics D: Applied Physics*, **2017**, 50, 22LT03	3	14
438	Fundamental limits on the electron mobility of GaO. *Journal of Physics Condensed Matter*, **2017**, 29, 234001	1.8	81
437	Growth of coherent BGaN films using BBr3 gas as a boron source in plasma assisted molecular beam epitaxy. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **2017**, 35, 041509	2.9	14
436	Phase transformations upon doping in WO. *Journal of Chemical Physics*, **2017**, 146, 214504	3.9	18
435	Computationally predicted energies and properties of defects in GaN. *Npj Computational Materials*, **2017**, 3,	10.9	141
434	Hole polarons and p-type doping in boron nitride polymorphs. *Physical Review B*, **2017**, 96,	3.3	14
433	Electrical compensation mechanism in fluorine-doped SnO2. *Applied Physics Letters*, **2017**, 111, 152107	3.4	4
432	Lack of quantum confinement in Ga2O3 nanolayers. *Physical Review B*, **2017**, 96,	3.3	27
431	Conditions for T2 resistivity from electron-electron scattering. *European Physical Journal B*, **2017**, 90, 1	1.2	7
430	First-principles characterization of native-defect-related optical transitions in ZnO. *Journal of Applied Physics*, **2017**, 122, 035704	2.5	67
429	Deep donor state of the copper acceptor as a source of green luminescence in ZnO. *Applied Physics Letters*, **2017**, 111, 042101	3.4	18
428	Hybrid functional study of native point defects and impurities in ZnGeN2. *Journal of Applied Physics*, **2017**, 122, 195701	2.5	17
427	Sub-band-gap absorption in Ga2O3. *Applied Physics Letters*, **2017**, 111, 182104	3.4	34
426	Electronic and protonic conduction in LaFeO3. *Journal of Materials Chemistry A*, **2017**, 5, 15367-15379	13	30
425	First-principles analysis of electron transport in BaSnO3. *Physical Review B*, **2017**, 95,	3.3	59
424	Band bowing and the direct-to-indirect crossover in random BAlN alloys. *Physical Review Materials*, **2017**, 1,	3.2	18
423	Hydrogen intercalation in MoS2. *Physical Review B*, **2016**, 94,	3.3	12
422	Effects of La 5d and 4f states on the electronic and optical properties of LaAlO3. *Physical Review B*, **2016**, 94,	3.3	7

421	Structural investigation of the bilayer iridate Sr3Ir2O7. *Physical Review B*, **2016**, 93,	3.3	27
420	Defects in AlN as candidates for solid-state qubits. *Physical Review B*, **2016**, 93,	3.3	35
419	Role of excited states in Shockley-Read-Hall recombination in wide-band-gap semiconductors. *Physical Review B*, **2016**, 93,	3.3	61
418	Energetic, spatial, and momentum character of the electronic structure at a buried interface: The two-dimensional electron gas between two metal oxides. *Physical Review B*, **2016**, 93,	3.3	22
417	Depth-Resolved Composition and Electronic Structure of Buried Layers and Interfaces in a LaNiO3/SrTiO3 Superlattice from Soft- and Hard- X-ray Standing-Wave Angle-Resolved Photoemission. *Journal of Electron Spectroscopy and Related Phenomena*, **2016**, 211, 70-81	1.7	8
416	Point defects, impurities, and small hole polarons in GdTiO3. *Physical Review B*, **2016**, 93,	3.3	18
415	Electron and chemical reservoir corrections for point-defect formation energies. *Physical Review B*, **2016**, 93,	3.3	42
414	Correct Implementation of Polarization Constants in Wurtzite Materials and Impact on III-Nitrides. *Physical Review X*, **2016**, 6,	9.1	49
413	Doping of Ga2O3 with transition metals. *Physical Review B*, **2016**, 94,	3.3	47
412	Role of oxygen vacancies in crystalline WO3. *Journal of Materials Chemistry C*, **2016**, 4, 6641-6648	7.1	65
411	Point-defect kinetics in □and □MgH2. *International Journal of Hydrogen Energy*, **2016**, 41, 5688-5692	6.7	9
410	Surprising stability of neutral interstitial hydrogen in diamond and cubic BN. *Journal of Physics Condensed Matter*, **2016**, 28, 06LT01	1.8	5
409	Identification of Microscopic Hole-Trapping Mechanisms in Nitride Semiconductors. *IEEE Electron Device Letters*, **2016**, 37, 154-156	4.4	6
408	**2016**,		1
407	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
406	Tutorial: Defects in semiconductors□Combining experiment and theory. *Journal of Applied Physics*, **2016**, 119, 181101	2.5	206
405	Band alignments between SmTiO3, GdTiO3, and SrTiO3. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **2016**, 34, 061102	2.9	5
404	Donor defects and small polarons on the TiO2(110) surface. *Journal of Applied Physics*, **2016**, 119, 181503	2.5	44

403	Iron as a source of efficient Shockley-Read-Hall recombination in GaN. *Applied Physics Letters*, **2016**, 109, 162107	3.4	50
402	BaSnO3 as a channel material in perovskite oxide heterostructures. *Applied Physics Letters*, **2016**, 108, 083501	3.4	61
401	Impact of Point Defects on Proton Conduction in Strontium Cerate. *Journal of Physical Chemistry C*, **2016**, 120, 9562-9568	3.8	10
400	Metal versus insulator behavior in ultrathin SrTiO3-based heterostructures. *Physical Review B*, **2016**, 94,	3.3	2
399	Impact of nitrogen and carbon on defect equilibrium in ZrO2. *Acta Materialia*, **2016**, 117, 286-292	8.4	9
398	Determination of the Mott-Hubbard gap in GdTiO3. *Physical Review B*, **2015**, 92,	3.3	11
397	Limitations to the room temperature mobility of two- and three-dimensional electron liquids in SrTiO3. *Applied Physics Letters*, **2015**, 106, 062102	3.4	41
396	Small hole polarons in rare-earth titanates. *Applied Physics Letters*, **2015**, 106, 232103	3.4	18
395	Brittle fracture toughnesses of GaN and AlN from first-principles surface-energy calculations. *Applied Physics Letters*, **2015**, 106, 212103	3.4	16
394	High optical power and low-efficiency droop blue light-emitting diodes using compositionally step-graded InGaN barrier. *Electronics Letters*, **2015**, 51, 1187-1189	1.1	17
393	Carbon-induced trapping levels in oxide dielectrics. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **2015**, 33, 01A120	2.9	10
392	First-principles theory of acceptors in nitride semiconductors. *Physica Status Solidi (B): Basic Research*, **2015**, 252, 900-908	1.3	90
391	First-principles calculations of indirect Auger recombination in nitride semiconductors. *Physical Review B*, **2015**, 92,	3.3	57
390	Defects as qubits in 3C□and 4H□SiC. *Physical Review B*, **2015**, 92,	3.3	67
389	Structural and electronic properties of SrZrO3 and Sr(Ti,Zr)O3 alloys. *Physical Review B*, **2015**, 92,	3.3	18
388	(InxGa1□)2O3 alloys for transparent electronics. *Physical Review B*, **2015**, 92,	3.3	68
387	First-principles study of surface charging in LaAlO3/SrTiO3 heterostructures. *Physical Review B*, **2015**, 92,	3.3	15
386	Free-carrier absorption in transparent conducting oxides: Phonon and impurity scattering in SnO2. *Physical Review B*, **2015**, 92,	3.3	28

385	Small polarons and point defects in barium cerate. *Physical Review B*, **2015**, 92,	3.3	26
384	Impact of electric-field dependent dielectric constants on two-dimensional electron gases in complex oxides. *Applied Physics Letters*, **2015**, 107, 183505	3.4	6
383	Effects of biaxial stress and layer thickness on octahedral tilts in LaNiO3. *Applied Physics Letters*, **2015**, 107, 261901	3.4	3
382	Exciton-dominated Dielectric Function of Atomically Thin MoS2 Films. *Scientific Reports*, **2015**, 5, 16996	4.9	114
381	Defects in Germanium **2015**, 1-23		2
380	Observation by resonant angle-resolved photoemission of a critical thickness for 2-dimensional electron gas formation in SrTiO3 embedded in GdTiO3. *Applied Physics Letters*, **2015**, 107, 231602	3.4	8
379	Sulfur doping of AlN and AlGaN for improved n-type conductivity. *Physica Status Solidi - Rapid Research Letters*, **2015**, 9, 462-465	2.5	11
378	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
377	Nitride-based high-electron-mobility transistor with single-layer InN for mobility-enhanced channel. *Applied Physics Express*, **2015**, 8, 024302	2.4	6
376	Brillouin zone and band structure of □Ga2O3. *Physica Status Solidi (B): Basic Research*, **2015**, 252, 828-832	1.3	176
375	Effects of hole localization on limiting p-type conductivity in oxide and nitride semiconductors. *Journal of Applied Physics*, **2014**, 115, 012014	2.5	52
374	Hybrid functional calculations of DX centers in AlN and GaN. *Physical Review B*, **2014**, 89,	3.3	97
373	Hydrogen passivation of impurities in Al(2)O(3). *ACS Applied Materials & Interfaces*, **2014**, 6, 4149-53	9.5	9
372	Oxide interfaces for novel electronic applications. *New Journal of Physics*, **2014**, 16, 025005	2.9	141
371	Interband and polaronic excitations in YTiO3 from first principles. *Physical Review B*, **2014**, 90,	3.3	18
370	Effects of In profile on simulations of InGaN/GaN multi-quantum-well light-emitting diodes. *Applied Physics Letters*, **2014**, 105, 083507	3.4	24
369	Direct view at excess electrons in TiO2 rutile and anatase. *Physical Review Letters*, **2014**, 113, 086402	7.4	300
368	Vacancies and small polarons in SrTiO3. *Physical Review B*, **2014**, 90,	3.3	156

367	Auger Recombination in GaAs from First Principles. *ACS Photonics*, **2014**, 1, 643-646	6.3	26
366	First-principles study of high-field-related electronic behavior of group-III nitrides. *Physical Review B* , **2014**, 90,	3.3	15
365	First-principles study of van der Waals interactions in MoS2 and MoO3. *Journal of Physics Condensed Matter*, **2014**, 26, 305502	1.8	37
364	First-principles theory of nonradiative carrier capture via multiphonon emission. *Physical Review B*, **2014**, 90,	3.3	168
363	Absolute surface energies of polar and nonpolar planes of GaN. *Physical Review B*, **2014**, 89,	3.3	76
362	High-voltage field effect transistors with wide-bandgap □Ga2O3 nanomembranes. *Applied Physics Letters*, **2014**, 104, 203111	3.4	242
361	Effects of strain on the band structure of group-III nitrides. *Physical Review B*, **2014**, 90,	3.3	73
360	Band alignments and polarization properties of BN polymorphs. *Applied Physics Express*, **2014**, 7, 031001	2.4	39
359	Elastic Constants and Pressure-Induced Effects in MoS2. *Journal of Physical Chemistry C*, **2014**, 118, 12073-12076	4.8	44
358	Effects of carbon on the electrical and optical properties of InN, GaN, and AlN. *Physical Review B*, **2014**, 89,	3.3	290
357	Hydrogen bonds in Al2O3 as dissipative two-level systems in superconducting qubits. *Scientific Reports*, **2014**, 4, 7590	4.9	33
356	Structure and energetics of LaAlO3 (001) surfaces. *Physical Review B*, **2014**, 90,	3.3	21
355	Origins of optical absorption and emission lines in AlN. *Applied Physics Letters*, **2014**, 105, 111104	3.4	94
354	First-principles study of vacancy-assisted impurity diffusion in ZnO. *APL Materials*, **2014**, 2, 096101	5.7	30
353	Band alignment at band-insulator/Mott-insulator interfaces. *Physica Status Solidi - Rapid Research Letters*, **2014**, 8, 577-582	2.5	5
352	Ferroelastic switching of doped zirconia: Modeling and understanding from first principles. *Physical Review B*, **2014**, 90,	3.3	20
351	Hydrogenated vacancies and hidden hydrogen in SrTiO3. *Physical Review B*, **2014**, 89,	3.3	33
350	Nature and evolution of the band-edge states in MoS2: From monolayer to bulk. *Physical Review B*, **2014**, 90,	3.3	110

349	Turning SrTiO3 into a Mott insulator. *Physical Review B*, **2014**, 90,	3.3	21
348	Hybrid functional calculations of point defects and hydrogen in SrZrO3. *Physical Review B*, **2014**, 89,	3.3	34
347	The role of native defects in the transport of charge and mass and the decomposition of Li4BN3H10. *Physical Chemistry Chemical Physics*, **2014**, 16, 25314-20	3.6	6
346	First-principles study of the mobility of SrTiO3. *Physical Review B*, **2014**, 90,	3.3	40
345	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
344	First-principles calculations for point defects in solids. *Reviews of Modern Physics*, **2014**, 86, 253-305	40.5	1431
343	Theory and Modeling of Oxide Semiconductors. *Semiconductors and Semimetals*, **2013**, 88, 1-37	0.6	5
342	Electronic structure of a single-layer InN quantum well in a GaN matrix. *Applied Physics Letters*, **2013**, 102, 102103	3.4	25
341	Polarization effects due to thickness fluctuations in nonpolar InGaN/GaN quantum wells. *Applied Physics Letters*, **2013**, 103, 073115	3.4	7
340	Impact of native defects in high-k dielectric oxides on GaN/oxide metal□oxide□emiconductor devices. *Physica Status Solidi (B): Basic Research*, **2013**, 250, 787-791	1.3	21
339	Native point defects in LaAlO3: A hybrid functional study. *Physical Review B*, **2013**, 88,	3.3	27
338	Ambipolar doping in SnO. *Applied Physics Letters*, **2013**, 103, 082118	3.4	80
337	Defects at Ge/oxide and III□/oxide interfaces. *Microelectronic Engineering*, **2013**, 109, 211-215	2.5	27
336	LiH as a Li+ and H□ion provider. *Solid State Ionics*, **2013**, 253, 53-56	3.3	6
335	Native point defects and dangling bonds in □Al2O3. *Journal of Applied Physics*, **2013**, 113, 044501	2.5	165
334	Enhanced Optical Absorption Due to Symmetry Breaking in TiO2(1□)S2x Alloys. *Journal of Physical Chemistry C*, **2013**, 117, 4189-4193	3.8	13
333	Effects of strain on the electron effective mass in GaN and AlN. *Applied Physics Letters*, **2013**, 102, 142105	3.4	45
332	Band offsets in complex-oxide thin films and heterostructures of SrTiO3/LaNiO3 and SrTiO3/GdTiO3 by soft and hard X-ray photoelectron spectroscopy. *Journal of Applied Physics*, **2013**, 113, 143704	2.5	28

331	Dual behavior of excess electrons in rutile TiO2. *Physica Status Solidi - Rapid Research Letters*, **2013**, 7, 199-203	2.5	126
330	Dangling bonds and vacancies in germanium. *Physical Review B*, **2013**, 87,	3.3	43
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