

Chris G. Van de Walle

List of Publications by Year in descending order

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522
papers

61,336
citations

1172

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h-index

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236
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554
all docs

554
docs citations

554
times ranked

38603
citing authors

#	ARTICLE	IF	CITATIONS
1	Defect tolerance in halide perovskites: A first-principles perspective. Journal of Applied Physics, 2022, 131, .	1.1	35
2	First-principles studies of diffusion in gallium oxide. , 2022, , .		0
3	Role of carbon and hydrogen in limiting n -type doping of monoclinic Al_2O_3 . Physical Review B, 2022, 105, .	1.1	18
4	Epitaxial ScAl_2N on GaN exhibits attractive high-K dielectric properties. Applied Physics Letters, 2022, 120, .	1.5	17
5	Anisotropic-strain-enhanced hole mobility in GaN by lattice matching to ZnGeN_2 and MgSiN_2 . Applied Physics Letters, 2022, 120, .	1.5	2
6	Defect Chemistry and Hydrogen Transport in La/Sr-Based Oxyhydrides. Journal of Physical Chemistry C, 2021, 125, 2250-2256.	1.5	3
7	Understanding carbon contamination in the proton-conducting zirconates and cerates. Physical Chemistry Chemical Physics, 2021, 23, 14205-14211.	1.3	3
8	Impact of dangling bonds on properties of h-BN. 2D Materials, 2021, 8, 024002.	2.0	6
9	Boron dangling bonds in a monolayer of hexagonal boron nitride. Journal of Applied Physics, 2021, 129, .	1.1	7
10	Adsorption and Diffusion of Aluminum on $\text{Ga}_2\text{O}_3(010)$ Surfaces. ACS Applied Materials & Interfaces, 2021, 13, 10650-10655.	4.0	7
11	A first-principles understanding of point defects and impurities in GaN. Journal of Applied Physics, 2021, 129, .	1.1	55
12	Thermodynamics of boron incorporation in BGaN. Physical Review Materials, 2021, 5, .	0.9	10
13	Finite-size correction for slab supercell calculations of materials with spontaneous polarization. Npj Computational Materials, 2021, 7, .	3.5	14
14	Minimizing hydrogen vacancies to enable highly efficient hybrid perovskites. Nature Materials, 2021, 20, 971-976.	13.3	92
15	Atomic scale investigation of aluminum incorporation, defects, and phase stability in $\text{Ga}_{1-x}\text{Al}_x\text{O}_3$ films. APL Materials, 2021, 9, .	2.2	35
16	Hydride Conductivity in Nitride Hydrides. ACS Applied Energy Materials, 2021, 4, 6348-6355.	2.5	6
17	Vibrational and vibronic structure of isolated point defects: The nitrogen-vacancy center in diamond. Physical Review B, 2021, 104, .	1.1	24
18	Materials and device simulations for silicon qubit design and optimization. MRS Bulletin, 2021, 46, 634-641.	1.7	6

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19	Hole Trapping at Acceptor Impurities and Alloying Elements in AlN. <i>Physica Status Solidi - Rapid Research Letters</i> , 2021, 15, 2100218.	1.2	3
20	First-principles study of electron transport in ScN. <i>Physical Review B</i> , 2021, 104, .	1.1	13
21	Piezoelectric effect and polarization switching in Al _{1-x} Sc _x N. <i>Journal of Applied Physics</i> , 2021, 130, .	1.1	15
22	Structural, electronic, and polarization properties of YN and LaN. <i>Physical Review Materials</i> , 2021, 5, .	0.9	4
23	Nonrad: Computing nonradiative capture coefficients from first principles. <i>Computer Physics Communications</i> , 2021, 267, 108056.	3.0	50
24	All-inorganic halide perovskites as candidates for efficient solar cells. <i>Cell Reports Physical Science</i> , 2021, 2, 100604.	2.8	28
25	Prospects for n-type conductivity in cubic boron nitride. <i>Applied Physics Letters</i> , 2021, 119, .	1.5	9
26	Surprising stability of polar (001) surfaces of the Mott insulator GdTiO ₃ . <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2021, 39, .	0.9	1
27	Incorporation of Si and Sn donors in $\hat{\Gamma}^2$ -Ga ₂ O ₃ through surface reconstructions. <i>Journal of Applied Physics</i> , 2021, 130, 185703.	1.1	7
28	Mg doping and diffusion in (010) $\hat{\Gamma}^2$ -Ga ₂ O ₃ films grown by plasma-assisted molecular beam epitaxy. <i>Journal of Applied Physics</i> , 2021, 130, .	1.1	10
29	Deep-Level Defects and Impurities in InGaN Alloys. <i>Physica Status Solidi (B): Basic Research</i> , 2020, 257, 1900534.	0.7	13
30	First-Principles Simulation of Carrier Recombination Mechanisms in Halide Perovskites. <i>Advanced Energy Materials</i> , 2020, 10, 1902830.	10.2	52
31	Anomalous Auger Recombination in PbSe. <i>Physical Review Letters</i> , 2020, 125, 037401.	2.9	16
32	First-principles calculations of hyperfine interaction, binding energy, and quadrupole coupling for shallow donors in silicon. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	17
33	Electronic structure and magneto-optical properties of silicon-nitrogen-vacancy complexes in diamond. <i>Physical Review B</i> , 2020, 102, .	1.1	10
34	First-principles surface energies for monoclinic Ga ₂ O ₃ and Al ₂ O ₃ and consequences for cracking of (Al _{1-x} Ga _x) ₂ O ₃ . <i>APL Materials</i> , 2020, 8, .	2.2	53
35	Radiative capture rates at deep defects from electronic structure calculations. <i>Physical Review B</i> , 2020, 102, .	1.1	14
36	Inflection points in the conduction-band structure of $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{BaSn} \langle \text{mml:mi} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mj} \rangle \langle \text{mml:mathvariant="normal"} \rangle \text{O} \langle \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 3 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \rangle .$ <i>Physical Review B</i> , 2020, 102, .	1.1	3

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37	Orientation-dependent band offsets between (Al _x Ga _{1-x}) ₂ O ₃ and Ga ₂ O ₃ . Applied Physics Letters, 2020, 117, .	1.5	24
38	Polarization properties at rocksalt/wurtzite oxide interfaces. Physical Review B, 2020, 102, .	1.1	4
39	Band alignments and polarization properties of the Zn-IV-nitrides. Journal of Materials Chemistry C, 2020, 8, 7890-7898.	2.7	19
40	Hidden role of Bi incorporation in nonradiative recombination in methylammonium lead iodide. Journal of Materials Chemistry A, 2020, 8, 12964-12967.	5.2	18
41	Prospects for high carrier mobility in the cubic germanates. Semiconductor Science and Technology, 2020, 35, 085030.	1.0	5
42	Role of Ga and In adatoms in the epitaxial growth of O_3 . Physical Review B, 2020, 102, .	1.1	11
43	First-principles study of transport in WO_3 . Physical Review B, 2020, 101, .		
44	Correctly Assessing Defect Tolerance in Halide Perovskites. Journal of Physical Chemistry C, 2020, 124, 6022-6027.	1.5	70
45	Effect of Titanium Induced Chemical Inhomogeneity on Crystal Structure, Electronic Structure, and Optical Properties of Wide Band Gap Ga_2O_3 . Crystal Growth and Design, 2020, 20, 1422-1433.	1.4	21
46	Spinning up quantum defects in 2D materials. Nature Materials, 2020, 19, 487-489.	13.3	18
47	Iodine interstitials as a cause of nonradiative recombination in hybrid perovskites. Physical Review B, 2020, 101, .	1.1	76
48	First-Principles Calculations 1. Springer Series in Materials Science, 2020, , 309-328.	0.4	0
49	Phonon- and charged-impurity-assisted indirect free-carrier absorption in Ga_2O_3 . Physical Review B, 2020, 101, .	1.1	11
50	Optimizing n -type doping of ZnGeN_2 and ZnSiN_2 . Physical Review B, 2020, 101, .	1.1	8
51	Unusual Formation of Point-Defect Complexes in the Ultrawide-Band-Gap Semiconductor ZnSiN_2 . Physical Review B, 2020, 101, .	1.1	8
52	First-principles study of electron-phonon interactions and transport in anatase TiO_2 . Physical Review B, 2019, 100, .	1.1	10
53	Impact of phonons and spin-orbit coupling on Auger recombination in InAs. Physical Review B, 2019, 100, .	1.1	2
54	Deep acceptors and their diffusion in Ga_2O_3 . APL Materials, 2019, 7, .	2.2	143

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55	First-principles study of bandgap bowing in BGaN alloys. Journal of Applied Physics, 2019, 126, 095706.	1.1	18
56	Limitations of In ₂ O ₃ as a transparent conducting oxide. Applied Physics Letters, 2019, 115, .	1.5	14
57	Dangling Bonds in Hexagonal Boron Nitride as Single-Photon Emitters. Physical Review Letters, 2019, 123, 127401.	2.9	68
58	Strategies for <i>p</i> -type doping of ZnGeN ₂ . Applied Physics Letters, 2019, 114, .	1.5	17
59	Hydrogen-Induced Degradation of NaMnO ₂ . Chemistry of Materials, 2019, 31, 5224-5228.	3.2	10
60	Electrical and optical properties of iron in GaN, AlN, and InN. Physical Review B, 2019, 99, .	1.1	30
61	Optimizing Proton Conductivity in Zirconates through Defect Engineering. ACS Applied Energy Materials, 2019, 2, 2611-2619.	2.5	25
62	First-principles study of antisite defects in perovskite stannates. Journal of Applied Physics, 2019, 126, 195701.	1.1	9
63	Carbon dimer defect as a source of the 4.1 eV luminescence in hexagonal boron nitride. Applied Physics Letters, 2019, 115, .	1.5	77
64	<i>Ab initio</i> study of enhanced thermal conductivity in ordered AlGaO ₃ alloys. Applied Physics Letters, 2019, 115, .	1.5	24
65	Giant polarization charge density at lattice-matched GaN/ScN interfaces. Applied Physics Letters, 2019, 115, .	1.5	15
66	Role of point defects in the electrical and optical properties of In ₂ O ₃ . Physical Review Materials, 2019, 3, .	0.9	37
67	Publisher's Note: Defects in AlN as candidates for solid-state qubits [Phys. Rev. B 93 , 161201(R) (2016)]. Physical Review B, 2018, 97, .	1.1	0
68	Comment on "Comparative study of <i>ab initio</i> nonradiative recombination rate calculations under different formalisms". Physical Review B, 2018, 97, .	1.1	11
69	Origins of <i>n</i> -type doping difficulties in perovskite stannates. Physical Review B, 2018, 97, .	1.1	41
70	First-Principles Calculations of Point Defects for Quantum Technologies. Annual Review of Materials Research, 2018, 48, 1-26.	4.3	93
71	Interfacial Cation-Defect Charge Dipoles in Stacked TiO ₂ /Al ₂ O ₃ Gate Dielectrics. ACS Applied Materials & Interfaces, 2018, 10, 5140-5146.	4.0	10
72	Publisher's Note: Hole polarons and <i>p</i> -type doping in boron nitride polymorphs [Phys. Rev. B 96 , 100102(R) (2017)]. Physical Review B, 2018, 97, .	1.1	2

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73	First-principles study of direct and indirect optical absorption in BaSnO ₃ . Applied Physics Letters, 2018, 112, 062106.	1.5	14
74	Posner molecules: from atomic structure to nuclear spins. Physical Chemistry Chemical Physics, 2018, 20, 12373-12380.	1.3	29
75	Linear Hyperfine Tuning of Donor Spins in Silicon Using Hydrostatic Strain. Physical Review Letters, 2018, 120, 167701.	2.9	34
76	Ultrawide-bandgap Semiconductors: Research Opportunities and Challenges. Advanced Electronic Materials, 2018, 4, 1600501.	2.6	839
77	Defect identification based on first-principles calculations for deep level transient spectroscopy. Applied Physics Letters, 2018, 113, .	1.5	51
78	Monolayer to Bulk Properties of Hexagonal Boron Nitride. Journal of Physical Chemistry C, 2018, 122, 25524-25529.	1.5	134
79	Sr ₃ Ir ₂ O ₇ F ₂ : Topochemical conversion of a relativistic Mott state into a spin-orbit driven band insulator. Physical Review B, 2018, 98, .	1.1	3
80	First-Principles Analysis of Radiative Recombination in Lead-Halide Perovskites. ACS Energy Letters, 2018, 3, 2329-2334.	8.8	81
81	Unexpectedly Strong Auger Recombination in Halide Perovskites. Advanced Energy Materials, 2018, 8, 1801027.	10.2	64
82	Three-Dimensional Spin Texture in Hybrid Perovskites and Its Impact on Optical Transitions. Journal of Physical Chemistry Letters, 2018, 9, 2903-2908.	2.1	50
83	Carrier-induced absorption as a mechanism for electrochromism in tungsten trioxide. MRS Communications, 2018, 8, 926-931.	0.8	9
84	Accurate and efficient band-offset calculations from density functional theory. Computational Materials Science, 2018, 151, 174-180.	1.4	56
85	Ion-Transport Engineering of Alkaline-Earth Hydrides for Hydride Electrolyte Applications. Chemistry of Materials, 2018, 30, 5878-5885.	3.2	15
86	Electron doping in Sr ₃ Ir ₂ O ₇ : Collapse of band gap and magnetic order. Physical Review B, 2018, 98, .	1.1	3
87	Native point defects and impurities in hexagonal boron nitride. Physical Review B, 2018, 97, .	1.1	200
88	Structural and electronic properties of Ga ₂ O ₃ -Al ₂ O ₃ alloys. Applied Physics Letters, 2018, 112, .	1.5	198
89	First-principles calculations of optical transitions at native defects and impurities in ZnO. , 2018, , .		1
90	Impact of point defects on electrochromism in WO ₃ . , 2018, , .		1

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91	Publisher's Note: Band bowing and the direct-to-indirect crossover in random BAlN alloys [Phys. Rev. Materials 1 (2017)]. Physical Review Materials, 2018, 2, .	0.9	0
92	Calcium as a nonradiative recombination center in InGaN. Applied Physics Express, 2017, 10, 021001.	1.1	19
93	<i>Ab initio</i> study of hydrogenic effective mass impurities in Si nanowires. Journal of Physics Condensed Matter, 2017, 29, 095303.	0.7	1
94	Controlling <i>n</i> -Type Doping in MoO ₃ . Chemistry of Materials, 2017, 29, 2563-2567.	3.2	74
95	Acceptor doping in the proton conductor SrZrO ₃ . Physical Chemistry Chemical Physics, 2017, 19, 11485-11491.	1.3	23
96	Identification of yellow luminescence centers in Be-doped GaN through pressure-dependent studies. Journal Physics D: Applied Physics, 2017, 50, 22LT03.	1.3	17
97	Fundamental limits on the electron mobility of <i>I</i> ² -Ga ₂ O ₃ . Journal of Physics Condensed Matter, 2017, 29, 234001.	0.7	99
98	Growth of coherent B ₂ GaN films using BBr ₃ gas as a boron source in plasma assisted molecular beam epitaxy. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2017, 35, .	0.9	16
99	Phase transformations upon doping in WO ₃ . Journal of Chemical Physics, 2017, 146, 214504.	1.2	25
100	Computationally predicted energies and properties of defects in GaN. Npj Computational Materials, 2017, 3, .	3.5	196
101	Hole polarons and <i>p</i> -type doping in boron nitride polymorphs. Physical Review B, 2017, 96, .	1.1	18
102	Electrical compensation mechanism in fluorine-doped SnO ₂ . Applied Physics Letters, 2017, 111, .	1.5	8
103	Lack of quantum confinement in Ga ₂ O ₃ nanolayers. Physical Review B, 2017, 96, .	1.1	36
104	Conditions for T ₂ resistivity from electron-electron scattering. European Physical Journal B, 2017, 90, 1.	0.6	12
105	First-principles characterization of native-defect-related optical transitions in ZnO. Journal of Applied Physics, 2017, 122, .	1.1	88
106	Deep donor state of the copper acceptor as a source of green luminescence in ZnO. Applied Physics Letters, 2017, 111, 042101.	1.5	26
107	Hybrid functional study of native point defects and impurities in ZnGeN ₂ . Journal of Applied Physics, 2017, 122, .	1.1	22
108	Sub-band-gap absorption in Ga ₂ O ₃ . Applied Physics Letters, 2017, 111, .	1.5	44

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109	Electronic and protonic conduction in LaFeO ₃ . Journal of Materials Chemistry A, 2017, 5, 15367-15379.	5.2	48
110	First-principles analysis of electron transport in BaSnO_3 . Physical Review B, 2017, 95, .	1.1	17
111	Band bowing and the direct-to-indirect crossover in random BAlN alloys. Physical Review Materials, 2017, 1, .	0.9	25
112	Auger recombination in InAs: Role of spin-orbit coupling and phonons. , 2016, , .		1
113	Gallium vacancy complexes as a cause of Shockley-Read-Hall recombination in III-nitride light emitters. Applied Physics Letters, 2016, 108, .	1.5	91
114	Tutorial: Defects in semiconductors – Combining experiment and theory. Journal of Applied Physics, 2016, 119, .	1.1	297
115	Band alignments between SmTiO ₃ , GdTIO ₃ , and SrTiO ₃ . Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2016, 34, .	0.9	6
116	Donor defects and small polarons on the TiO ₂ (110) surface. Journal of Applied Physics, 2016, 119, .	1.1	51
117	Iron as a source of efficient Shockley-Read-Hall recombination in GaN. Applied Physics Letters, 2016, 109, .	1.5	64
118	BaSnO ₃ as a channel material in perovskite oxide heterostructures. Applied Physics Letters, 2016, 108, .	1.5	81
119	Impact of Point Defects on Proton Conduction in Strontium Cerate. Journal of Physical Chemistry C, 2016, 120, 9562-9568.	1.5	11
120	Metal versus insulator behavior in ultrathin SrTiO_3 -based heterostructures. Physical Review B, 2016, 94, .	1.1	2
121	Impact of nitrogen and carbon on defect equilibrium in ZrO ₂ . Acta Materialia, 2016, 117, 286-292.	3.8	9
122	Hydrogen intercalation in MoS_2 . Physical Review B, 2016, 94, .	1.1	15
123	Effects of La 5d and 4f states on the electronic and optical properties of LaAlO ₃ . Physical Review B, 2016, 94, .	1.1	14
124	Structural investigation of the bilayer iridate Sr_3O_7 . Physical Review B, 2016, 93, .	1.1	35
125	Defects in AlN as candidates for solid-state qubits. Physical Review B, 2016, 93, .	1.1	50
126	Role of excited states in Shockley-Read-Hall recombination in wide-band-gap semiconductors. Physical Review B, 2016, 93, .	1.1	89

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127	Energetic, spatial, and momentum character of the electronic structure at a buried interface: The two-dimensional electron gas between two metal oxides. <i>Physical Review B</i> , 2016, 93, .	1.1	29
128	Depth-Resolved Composition and Electronic Structure of Buried Layers and Interfaces in a LaNiO ₃ /SrTiO ₃ Superlattice from Soft- and Hard- X-ray Standing-Wave Angle-Resolved Photoemission. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2016, 211, 70-81.	0.8	9
129	Point defects, impurities, and small hole polarons in CdTiO_3 . <i>Physical Review B</i> , 2016, 93, .	1.1	22
130	Electron and chemical reservoir corrections for point-defect formation energies. <i>Physical Review B</i> , 2016, 93, .	1.1	50
131	Correct Implementation of Polarization Constants in Wurtzite Materials and Impact on III-Nitrides. <i>Physical Review X</i> , 2016, 6, .	2.8	81
132	Doping of Ga_2O_3 with transition metals. <i>Physical Review B</i> , 2016, 94, .	1.1	61
133	Role of oxygen vacancies in crystalline WO_3 . <i>Journal of Materials Chemistry C</i> , 2016, 4, 6641-6648.	2.7	95
134	Point-defect kinetics in H^\pm - and H^3 -MgH ₂ . <i>International Journal of Hydrogen Energy</i> , 2016, 41, 5688-5692.	3.8	11
135	Surprising stability of neutral interstitial hydrogen in diamond and cubic BN. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 06LT01.	0.7	7
136	Identification of Microscopic Hole-Trapping Mechanisms in Nitride Semiconductors. <i>IEEE Electron Device Letters</i> , 2016, 37, 154-156.	2.2	7
137	First-principles theory of acceptors in nitride semiconductors. <i>Physica Status Solidi (B): Basic Research</i> , 2015, 252, 900-908.	0.7	115
138	First-principles calculations of indirect Auger recombination in nitride semiconductors. <i>Physical Review B</i> , 2015, 92, .	1.1	77
139	Defects as qubits in SrTiO_3 . <i>Physical Review B</i> , 2015, 92, .	1.1	88
140	Structural and electronic properties of SrZrO_3 alloys. <i>Physical Review B</i> , 2015, 92, .	1.1	27
141	LaAlO_3 for transparent electronics. <i>Physical Review B</i> , 2015, 92, .	1.1	30
142	First-principles study of surface charging in LaAlO_3 . <i>Physical Review B</i> , 2015, 92, .	1.1	34
143	Free-carrier absorption in transparent conducting oxides: Phonon and impurity scattering in SnO_2 . <i>Physical Review B</i> , 2015, 92, .	1.1	34
144	Small polarons and point defects in barium cerate. <i>Physical Review B</i> , 2015, 92, .	1.1	33

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145	Impact of electric-field dependent dielectric constants on two-dimensional electron gases in complex oxides. Applied Physics Letters, 2015, 107, .	1.5	10
146	Effects of biaxial stress and layer thickness on octahedral tilts in LaNiO ₃ . Applied Physics Letters, 2015, 107, 261901.	1.5	3
147	Exciton-dominated Dielectric Function of Atomically Thin MoS ₂ Films. Scientific Reports, 2015, 5, 16996.	1.6	155
148	Observation by resonant angle-resolved photoemission of a critical thickness for 2-dimensional electron gas formation in SrTiO ₃ embedded in GdTiO ₃ . Applied Physics Letters, 2015, 107, 231602.	1.5	9
149	Sulfur doping of AlN and AlGaN for improved n-type conductivity. Physica Status Solidi - Rapid Research Letters, 2015, 9, 462-465.	1.2	12
150	Tuning bad metal and non-Fermi liquid behavior in a Mott material: Rare-earth nickelate thin films. Science Advances, 2015, 1, e1500797.	4.7	99
151	Nitride-based high-electron-mobility transistor with single-layer InN for mobility-enhanced channel. Applied Physics Express, 2015, 8, 024302.	1.1	8
152	Brillouin zone and band structure of $\text{In}_2\text{Ga}_2\text{O}_3$. Physica Status Solidi (B): Basic Research, 2015, 252, 828-832.	0.7	242
153	Determination of the Mott-Hubbard gap in GdTiO ₃ . Physical Review B, 2015, 92, .	1.1	15
154	Limitations to the room temperature mobility of two- and three-dimensional electron liquids in SrTiO ₃ . Applied Physics Letters, 2015, 106, .	1.5	51
155	Small hole polarons in rare-earth titanates. Applied Physics Letters, 2015, 106, .	1.5	22
156	Brittle fracture toughnesses of GaN and AlN from first-principles surface-energy calculations. Applied Physics Letters, 2015, 106, .	1.5	21
157	High optical power and low efficiency droop blue light emitting diodes using compositionally step-graded InGaN barrier. Electronics Letters, 2015, 51, 1187-1189.	0.5	21
158	Carbon-induced trapping levels in oxide dielectrics. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2015, 33, .	0.9	12
159	Structure and energetics of LaAlO_3 surfaces. Physical Review B, 2014, 90, .	2.0	20
160	Auger recombination in light-emitting materials. , 2014, , .		0
161	Origins of optical absorption and emission lines in AlN. Applied Physics Letters, 2014, 105, .	1.5	127
162	First-principles study of vacancy-assisted impurity diffusion in ZnO. APL Materials, 2014, 2, 096101.	2.2	35

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163	Band alignment at band-insulator/Mott-insulator interfaces. Physica Status Solidi - Rapid Research Letters, 2014, 8, 577-582.	1.2	5
164	Ferroelastic switching of doped zirconia: Modeling and understanding from first principles. Physical Review B, 2014, 90, .	1.1	28
165	Hydrogenated vacancies and hidden hydrogen in SrTiO ₃ . Physical Review B, 2014, 89, .	1.1	36
166	Nature and evolution of the band-edge states in MoS ₂ . From monolayer to bulk. Physical Review B, 2014, 90, .	1.1	38
167	Turning SrTiO ₃ a Mott insulator. Physical Review B, 2014, 90, .	1.1	25
168	Hybrid functional calculations of point defects and hydrogen in SrZrO ₃ . Physical Review B, 2014, 89, .	1.1	40
169	The role of native defects in the transport of charge and mass and the decomposition of Li ₄ BN ₃ H ₁₀ . Physical Chemistry Chemical Physics, 2014, 16, 25314-25320.	1.3	6
170	First-principles study of the mobility of SrTiO ₃ . Physical Review B, 2014, 90, .	1.1	45
171	First-principles theory of the luminescence lineshape for the triplet transition in diamond NV centres. New Journal of Physics, 2014, 16, 073026.	1.2	183
172	First-principles calculations for point defects in solids. Reviews of Modern Physics, 2014, 86, 253-305.	16.4	1,967
173	Effects of hole localization on limiting <i>p</i> -type conductivity in oxide and nitride semiconductors. Journal of Applied Physics, 2014, 115, 012014.	1.1	55
174	Hybrid functional calculations of D ₁₉ in AlN and GaN. Physical Review B, 2014, 89, .	1.1	19
175	Hydrogen Passivation of Impurities in Al ₂ O ₃ . ACS Applied Materials & Interfaces, 2014, 6, 4149-4153.	4.0	12
176	Oxide interfaces for novel electronic applications. New Journal of Physics, 2014, 16, 025005.	1.2	157
177	Interband and polaronic excitations in YTiO ₃ first principles. Physical Review B, 2014, 90, .	1.1	25
178	Effects of In profile on simulations of InGaN/GaN multi-quantum-well light-emitting diodes. Applied Physics Letters, 2014, 105, .	1.5	28
179	Direct View at Excess Electrons in TiO ₂ and Anatase. Physical Review Letters, 2014, 113, 086402.	1.1	17
180	Vacancies and small polarons in SrTiO ₃ . Physical Review B, 2014, 90, .	1.1	192

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181	Auger Recombination in GaAs from First Principles. ACS Photonics, 2014, 1, 643-646.	3.2	30
182	First-principles study of high-field-related electronic behavior of group-III nitrides. Physical Review B, 2014, 90, .	1.1	20
183	First-principles study of van der Waals interactions in MoS ₂ and MoO ₃ . Journal of Physics Condensed Matter, 2014, 26, 305502.	0.7	45
184	First-principles theory of nonradiative carrier capture via multiphonon emission. Physical Review B, 2014, 90, .	1.1	263
185	Absolute surface energies of polar and nonpolar planes of GaN. Physical Review B, 2014, 89, .	1.1	89
186	High-voltage field effect transistors with wide-bandgap α -Ga ₂ O ₃ nanomembranes. Applied Physics Letters, 2014, 104, .	1.5	288
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