Chris G. Van de Walle

List of Publications by Year
in descending order

522	61,336	997 114	1009 236
papers	citations	h-index	g-index

554	554	554	33998
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Fundamentals of zinc oxide as a semiconductor. Reports on Progress in Physics, 2009, 72, 126501.	20.1	3,166
2	First-principles calculations for defects and impurities: Applications to III-nitrides. Journal of Applied Physics, 2004, 95, 3851-3879.	2.5	2,695
3	Hydrogen as a Cause of Doping in Zinc Oxide. Physical Review Letters, 2000, 85, 1012-1015.	7.8	2,051
4	Native point defects in ZnO. Physical Review B, 2007, 76, .	3.2	2,051
5	Band lineups and deformation potentials in the model-solid theory. Physical Review B, 1989, 39, 1871-1883.	3.2	2,007
6	First-principles calculations for point defects in solids. Reviews of Modern Physics, 2014, 86, 253-305.	45.6	1,967
7	First-principles study of native point defects in ZnO. Physical Review B, 2000, 61, 15019-15027.	3.2	1,552
8	Theoretical calculations of heterojunction discontinuities in the Si/Ge system. Physical Review B, 1986, 34, 5621-5634.	3.2	1,282
9	Universal alignment of hydrogen levels in semiconductors, insulators and solutions. Nature, 2003, 423, 626-628.	27.8	1,111
10	FullyAb InitioFinite-Size Corrections for Charged-Defect Supercell Calculations. Physical Review Letters, 2009, 102, 016402.	7.8	1,093
11	Gallium vacancies and the yellow luminescence in GaN. Applied Physics Letters, 1996, 69, 503-505.	3.3	1,063
12	Oxygen vacancies in ZnO. Applied Physics Letters, 2005, 87, 122102.	3.3	1,015
13	Ultrawideâ€Bandgap Semiconductors: Research Opportunities and Challenges. Advanced Electronic Materials, 2018, 4, 1600501.	5.1	839
14	Atomic geometry and electronic structure of native defects in GaN. Physical Review B, 1994, 50, 8067-8070.	3.2	736
15	Oxygen vacancies and donor impurities in Î²-Ga2O3. Applied Physics Letters, 2010, 97, .	3.3	733
16	Hydrogen multicentre bonds. Nature Materials, 2007, 6, 44-47.	27.5	658
17	Density-functional calculations for III-V nitrides using the local-density approximation and the generalized gradient approximation. Physical Review B, 1999, 59, 5521-5535.	3.2	641
18	Theoretical study of band offsets at semiconductor interfaces. Physical Review B, 1987, 35, 8154-8165.	3.2	606

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19	Quantum computing with defects. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 8513-8518.	7.1	588
20	Hybrid functional studies of the oxygen vacancy in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu Physical Review B, 2010, 81, .	3.2	554
21	Carbon impurities and the yellow luminescence in GaN. Applied Physics Letters, 2010, 97, .	3.3	531
22	Theory of hydrogen diffusion and reactions in crystalline silicon. Physical Review B, 1989, 39, 10791-10808.	3.2	494
23	Indirect Auger recombination as a cause of efficiency droop in nitride light-emitting diodes. Applied Physics Letters, 2011, 98, .	3.3	447
24	Heterojunction band offset engineering. Surface Science Reports, 1996, 25, 1-140.	7.2	445
25	Role of self-trapping in luminescence and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>p</mml:mi></mml:math>-type conductivity of wide-band-gap oxides. Physical Review B, 2012, 85, .	3.2	440
26	Hydrogen in GaN: Novel Aspects of a Common Impurity. Physical Review Letters, 1995, 75, 4452-4455.	7.8	421
27	Effects of strain on band structure and effective masses in MoS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 86, .	3.2	405
28	Electrostatic interactions between charged defects in supercells. Physica Status Solidi (B): Basic Research, 2011, 248, 1067-1076.	1.5	395
29	Direct View at Excess Electrons in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>TiO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn> and Anatase. Physical Review Letters, 2014, 113, 086402.	7.8	373
30	Why nitrogen cannot lead to p-type conductivity in ZnO. Applied Physics Letters, 2009, 95, .	3.3	364
31	Effects of carbon on the electrical and optical properties of InN, GaN, and AlN. Physical Review B, 2014, 89, .	3.2	357
32	Sources of Electrical Conductivity in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>SnO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2008, 101, 055502.	7.8	352
33	Hydrogen-related defects in ZnO studied by infrared absorption spectroscopy. Physical Review B, 2002, 66, .	3.2	329
34	Auger recombination rates in nitrides from first principles. Applied Physics Letters, 2009, 94, .	3.3	323
35	Band bowing and band alignment in InGaN alloys. Applied Physics Letters, 2010, 96, .	3.3	319
36	Effects of cationdstates on the structural and electronic properties of III-nitride and II-oxide wide-band-gap semiconductors. Physical Review B, 2006, 74, .	3.2	318

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37	New insights into the role of native point defects in ZnO. Journal of Crystal Growth, 2006, 287, 58-65.	1.5	315
38	Role of hydrogen in doping of GaN. Applied Physics Letters, 1996, 68, 1829-1831.	3.3	304
39	Energies of various configurations of hydrogen in silicon. Physical Review B, 1994, 49, 4579-4585.	3.2	301
40	Energetics and electronic structure of stacking faults in AlN, GaN, and InN. Physical Review B, 1998, 57, R15052-R15055.	3.2	298
41	Tutorial: Defects in semiconductorsâ€"Combining experiment and theory. Journal of Applied Physics, 2016, 119, .	2.5	297
42	High-voltage field effect transistors with wide-bandgap Î²-Ga2O3 nanomembranes. Applied Physics Letters, 2014, 104, .	3.3	288
43	First-principles calculations of solubilities and doping limits: Li, Na, and N in ZnSe. Physical Review B, 1993, 47, 9425-9434.	3.2	282
44	Native defects and self-compensation in ZnSe. Physical Review B, 1992, 45, 10965-10978.	3.2	273
45	Electronic structure and phase stability ofGaAs1â^'xNxalloys. Physical Review B, 1995, 51, 10568-10571.	3.2	273
46	Experimental electronic structure of In₂O₃and Ga₂O₃. New Journal of Physics, 2011, 13, 085014.	2.9	273
47	Diffusivity of native defects in GaN. Physical Review B, 2004, 69, .	3.2	265
48	First-principles theory of nonradiative carrier capture via multiphonon emission. Physical Review B, 2014, 90, .	3.2	263
49	Hybrid functional investigations of band gaps and band alignments for AlN, GaN, InN, and InGaN. Journal of Chemical Physics, 2011, 134, 084703.	3.0	256
50	Microscopic origins of surface states on nitride surfaces. Journal of Applied Physics, 2007, 101, 081704.	2.5	248
51	Brillouin zone and band structure of Î²â€Ga₂O₃. Physica Status Solidi (B): Basic Research, 2015, 252, 828-832.	1.5	242
52	Defect analysis and engineering in ZnO. Physica B: Condensed Matter, 2001, 308-310, 899-903.	2.7	237
53	Hydrogenated cation vacancies in semiconducting oxides. Journal of Physics Condensed Matter, 2011, 23, 334212.	1.8	237
54	Interactions of hydrogen with native defects in GaN. Physical Review B, 1997, 56, R10020-R10023.	3.2	234

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55	Theory of Hydrogen Diffusion and Reactions in Crystalline Silicon. Physical Review Letters, 1988, 60, 2761-2764.	7.8	233
56	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	233
57	First-principles calculations of hyperfine parameters. Physical Review B, 1993, 47, 4244-4255.	3.2	231
58	Shallow versus Deep Nature of Mg Acceptors in Nitride Semiconductors. Physical Review Letters, 2012, 108, 156403.	7.8	230
59	First-Principles Surface Phase Diagram for Hydrogen on GaN Surfaces. Physical Review Letters, 2002, 88, 066103.	7.8	229
60	Theoretical investigation of native defects, impurities, and complexes in aluminum nitride. Physical Review B, 2002, 65, .	3.2	225
61	Defect Formation Energies without the Band-Gap Problem: Combining Density-Functional Theory and the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:math>Approach for the Silicon Self-Interstitial. Physical Review Letters, 2009, 102, 026402.	7.8	218
62	Electrostatic carrier doping of GdTiO3/SrTiO3 interfaces. Applied Physics Letters, 2011, 99, .	3.3	214
63	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.	3.2	209
64	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.	1.6	206
65	Large band gap bowing of InxGa1â^'xN alloys. Applied Physics Letters, 1998, 72, 2725-2726.	3.3	204
66	Theory of doping and defects in IIIâ€“V nitrides. Journal of Crystal Growth, 1998, 189-190, 505-510.	1.5	202
67	Native point defects and impurities in hexagonal boron nitride. Physical Review B, 2018, 97, .	3.2	200
68	Native point defects and dangling bonds in Î±-Al2O3. Journal of Applied Physics, 2013, 113, .	2.5	199
69	Optical characterization and band offsets in ZnSe-ZnSxSe1â^'xstrained-layer superlattices. Physical Review B, 1988, 38, 1417-1426.	3.2	198
70	Structural and electronic properties of Ga2O3-Al2O3 alloys. Applied Physics Letters, 2018, 112, .	3.3	198
71	Computationally predicted energies and properties of defects in GaN. Npj Computational Materials, 2017, 3, .	8.7	196
72	â€˜â€˜Absoluteâ€™â€™ deformation potentials: Formulation andab initiocalculations for semiconductors. Physical Review Letters, 1989, 62, 2028-2031.	7.8	192

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73	Vacancies and small polarons in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2014, 90, .	3.2	192
74	First-Principles Calculations of Luminescence Spectrum Line Shapes for Defects in Semiconductors: The Example of GaN and ZnO. Physical Review Letters, 2012, 109, 267401.	7.8	187
75	Origins of Fermi-level pinning on GaN and InN polar and nonpolar surfaces. Europhysics Letters, 2006, 76, 305-311.	2.0	183
76	First-principles theory of the luminescence lineshape for the triplet transition in diamond NV centres. New Journal of Physics, 2014, 16, 073026.	2.9	183
77	Energy levels of isolated interstitial hydrogen in silicon. Physical Review B, 2001, 64, .	3.2	179
78	Indium incorporation and emission properties of nonpolar and semipolar InGaN quantum wells. Applied Physics Letters, 2012, 100, .	3.3	168
79	Hydrogen doping in indium oxide: Anab initiostudy. Physical Review B, 2009, 80, .	3.2	167
80	Interplay of polarization fields and Auger recombination in the efficiency droop of nitride light-emitting diodes. Applied Physics Letters, 2012, 101, .	3.3	165
81	Electronic properties of the (100) (Si)/(Ge) strained-layer superlattices. Physical Review B, 1988, 38, 13237-13245.	3.2	160
82	Mechanism of Visibleâ€Light Photocatalysis in Nitrogenâ€Doped TiO₂. Advanced Materials, 2011, 23, 2343-2347.	21.0	160
83	Polarization-Driven Topological Insulator Transition in a<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>GaN</mml:mi><mml:mo>/</mml:mo><mml:mi>InN</mml:mi><mml:mo>/</mml:mo><mml:mi>GaN</mml:mi></mml:math>Well. Physical Review Letters, 2012, 109, 186803.	7.8	158
84	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.	1.6	157
85	Measurement and Control of Single Nitrogen-Vacancy Center Spins above 600ÂK. Physical Review X, 2012, 2, .	8.9	157
86	First-Principles Optical Spectra for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>F</mml:mi></mml:math>Centers in MgO. Physical Review Letters, 2012, 108, 126404.	7.8	157
87	Oxide interfaces for novel electronic applications. New Journal of Physics, 2014, 16, 025005.	2.9	157
88	Exciton-dominated Dielectric Function of Atomically Thin MoS2 Films. Scientific Reports, 2015, 5, 16996.	3.3	155
89	Metastability of Oxygen Donors in AlGaN. Physical Review Letters, 1998, 80, 4008-4011.	7.8	154
90	Microscopic structure of the hydrogen-boron complex in crystalline silicon. Physical Review B, 1989, 39, 10809-10824.	3.2	152

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91	Strain effects in group-III nitrides: Deformation potentials for AlN, GaN, and InN. Applied Physics Letters, 2009, 95, .	3.3	151
92	HYDROGEN IN SEMICONDUCTORS. Annual Review of Materials Research, 2006, 36, 179-198.	9.3	150
93	Doping of AlxGa1â^'xN. Applied Physics Letters, 1998, 72, 459-461.	3.3	149
94	Native defects in Al2O3 and their impact on III-V/Al2O3 metal-oxide-semiconductor-based devices. Journal of Applied Physics, 2011, 109, .	2.5	149
95	Mechanisms of dopant impurity diffusion in silicon. Physical Review B, 1989, 40, 5484-5496.	3.2	148
96	Origin and passivation of fixed charge in atomic layer deposited aluminum oxide gate insulators on chemically treated InGaAs substrates. Applied Physics Letters, 2010, 96, .	3.3	148
97	The electronic structure of Î²-Ga2O3. Applied Physics Letters, 2010, 97, .	3.3	146
98	Tin dioxide from first principles: Quasiparticle electronic states and optical properties. Physical Review B, 2011, 83, .	3.2	145
99	Phonon-Assisted Optical Absorption in Silicon from First Principles. Physical Review Letters, 2012, 108, 167402.	7.8	143
100	Deep acceptors and their diffusion in Ga2O3. APL Materials, 2019, 7, .	5.1	143
101	DX-center formation in wurtzite and zinc-blendeAlxGa1â^'xN. Physical Review B, 1998, 57, R2033-R2036.	3.2	141
102	Dual behavior of excess electrons in rutile TiO₂. Physica Status Solidi - Rapid Research Letters, 2013, 7, 199-203.	2.4	140
103	Hydrogen passivation effect in nitrogen-doped ZnO thin films. Applied Physics Letters, 2005, 86, 122107.	3.3	139
104	Nature and evolution of the band-edge states in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mm From monolayer to bulk. Physical Review B, 2014, 90, .	3.2	138
105	Role of native defects in wide-band-gap semiconductors. Physical Review Letters, 1991, 66, 648-651.	7.8	136
106	Role of nitrogen vacancies in the luminescence of Mg-doped GaN. Applied Physics Letters, 2012, 100, .	3.3	136
107	Small valence-band offsets at GaN/InGaN heterojunctions. Applied Physics Letters, 1997, 70, 2577-2579.	3.3	134
108	Monolayer to Bulk Properties of Hexagonal Boron Nitride. Journal of Physical Chemistry C, 2018, 122, 25524-25529.	3.1	134

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109	First-principles studies of beryllium doping of GaN. Physical Review B, 2001, 63, .	3.2	133
110	Absolute deformation potentials and band alignment of wurtzite ZnO, MgO, and CdO. Physical Review B, 2007, 75, .	3.2	128
111	Dangling-bond defects and hydrogen passivation in germanium. Applied Physics Letters, 2007, 91, .	3.3	127
112	Origins of optical absorption and emission lines in AlN. Applied Physics Letters, 2014, 105, .	3.3	127
113	Hybrid functional calculations of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>D</mml:mi><mml:mi>X</mml:mi></mml:mrow></mml in AlN and GaN. Physical Review B, 2014, 89, .	3.2	119
114	Quantitative analysis of the polarization fields and absorption changes in InGaN/GaN quantum wells with electroabsorption spectroscopy. Applied Physics Letters, 2002, 81, 490-492.	3.3	116
115	Firstâ€principles theory of acceptors in nitride semiconductors. Physica Status Solidi (B): Basic Research, 2015, 252, 900-908.	1.5	115
116	Effects of doping on the lattice parameter of SrTiO3. Applied Physics Letters, 2012, 100, .	3.3	114
117	Inverted order of acceptor and donor levels of monatomic hydrogen in silicon. Physical Review Letters, 1994, 73, 130-133.	7.8	112
118	Energetics and Vibrational Frequencies of InterstitialH2Molecules in Semiconductors. Physical Review Letters, 1998, 80, 2177-2180.	7.8	109
119	Interactions between hydrogen impurities and vacancies in Mg and Al: A comparative analysis based on density functional theory. Physical Review B, 2009, 80, .	3.2	109
120	Free-carrier absorption in nitrides from first principles. Physical Review B, 2010, 81, .	3.2	109
121	Temperature and carrier-density dependence of Auger and radiative recombination in nitride optoelectronic devices. New Journal of Physics, 2013, 15, 125006.	2.9	109
122	LDAâ€‰+â€‰U and hybrid functional calculations for defects in ZnO, SnO₂, and TiO₂. Physica Status Solidi (B): Basic Research, 2011, 248, 799-804.	1.5	108
123	Structure and properties of hydrogen-impurity pairs in elemental semiconductors. Physical Review Letters, 1989, 62, 1884-1887.	7.8	107
124	Fluorine-silicon reactions and the etching of crystalline silicon. Physical Review Letters, 1988, 61, 1867-1870.	7.8	102
125	Effects of strain on the band structure of group-III nitrides. Physical Review B, 2014, 90, .	3.2	100
126	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow><mml:mo>(</mml:mo> for transparent electronics. Physical Review B, 2015, 92, .	3.2	100

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127	Clean and As-Covered Zinc-Blende GaN (001) Surfaces: Novel Surface Structures and Surfactant Behavior. Physical Review Letters, 1998, 80, 3097-3100.	7.8	99
128	Interactions between nitrogen, hydrogen, and gallium vacancies inGaAs1â^'xNxalloys. Physical Review B, 2003, 67, .	3.2	99
129	Tuning bad metal and non-Fermi liquid behavior in a Mott material: Rare-earth nickelate thin films. Science Advances, 2015, 1, e1500797.	10.3	99
130	Fundamental limits on the electron mobility ofÎ²-Ga₂O₃. Journal of Physics Condensed Matter, 2017, 29, 234001.	1.8	99
131	Mechanisms of equilibrium and nonequilibrium diffusion of dopants in silicon. Physical Review Letters, 1989, 62, 1049-1052.	7.8	96
132	Impact of carbon and nitrogen impurities in high-Îº dielectrics on metal-oxide-semiconductor devices. Applied Physics Letters, 2013, 102, .	3.3	96
133	First-principles investigation of visible light emission from silicon-based materials. Physical Review Letters, 1993, 70, 1116-1119.	7.8	95
134	Chemical trends for acceptor impurities in GaN. Journal of Applied Physics, 1999, 85, 3003-3005.	2.5	95
135	Effects of Hydrogen on the Electronic Properties of Dilute GaAsN Alloys. Physical Review Letters, 2002, 89, 086403.	7.8	95
136	Role of oxygen vacancies in crystalline WO₃. Journal of Materials Chemistry C, 2016, 4, 6641-6648.	5.5	95
137	Oxidation and the origin of the two-dimensional electron gas in AlGaN/GaN heterostructures. Journal of Applied Physics, 2010, 107, .	2.5	94
138	Ambipolar doping in SnO. Applied Physics Letters, 2013, 103, .	3.3	94
139	Fundamental limits on optical transparency of transparent conducting oxides: Free-carrier absorption in SnO2. Applied Physics Letters, 2012, 100, .	3.3	93
140	First-Principles Calculations of Point Defects for Quantum Technologies. Annual Review of Materials Research, 2018, 48, 1-26.	9.3	93
141	Role of charged defects and impurities in kinetics of hydrogen storage materials: A first-principles study. Physical Review B, 2007, 76, .	3.2	92
142	Minimizing hydrogen vacancies to enable highly efficient hybrid perovskites. Nature Materials, 2021, 20, 971-976.	27.5	92
143	Gallium vacancy complexes as a cause of Shockley-Read-Hall recombination in III-nitride light emitters. Applied Physics Letters, 2016, 108, .	3.3	91
144	Acceptor doping in ZnSe versus ZnTe. Applied Physics Letters, 1993, 63, 1375-1377.	3.3	90

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145	Comment on â€˜â€˜Reduction of hot electron degradation in metal oxide semiconductor transistors by deuterium processingâ€™â€™ [Appl. Phys. Lett. 68, 2526 (1996)]. Applied Physics Letters, 1996, 69, 2441-2441.	3.3	90
146	Absolute surface energies of polar and nonpolar planes of GaN. Physical Review B, 2014, 89, .	3.2	89
147	Role of excited states in Shockley-Read-Hall recombination in wide-band-gap semiconductors. Physical Review B, 2016, 93, .	3.2	89
148	The role of oxygen-related defects and hydrogen impurities in HfO2 and ZrO2. Microelectronic Engineering, 2011, 88, 1452-1456.	2.4	88
149	Controlling the density of the two-dimensional electron gas at the SrTiO3/LaAlO3interface. Physical Review B, 2012, 86, .	3.2	88
150	Defects as qubits in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mn>3</mml:mn><mml:mi>C</mml:mi><mml:mtext>â^’</mml:mtext></mml:mtext><mml:mn>4</mml:mn><mml:mi>H</mml:mi><mml:mtext>â^’</mml:mtext><mm Physical Review B, 2015, 92, .	3.2	88
151	First-principles characterization of native-defect-related optical transitions in ZnO. Journal of Applied Physics, 2017, 122, .	2.5	88
152	Microscopic structure of the hydrogen-phosphorus complex in crystalline silicon. Physical Review B, 1990, 41, 3885-3888.	3.2	87
153	Strategies for Controlling the Conductivity of Wide-Band-Gap Semiconductors. Physica Status Solidi (B): Basic Research, 2002, 229, 221-228.	1.5	87
154	Effects of impurities on the lattice parameters of GaN. Physical Review B, 2003, 68, .	3.2	87
155	Shallow donor state of hydrogen in indium nitride. Applied Physics Letters, 2003, 82, 592-594.	3.3	86
156	Surface reconstructions on InN and GaN polar and nonpolar surfaces. Surface Science, 2007, 601, L15-L18.	1.9	85
157	Causes of incorrect carrier-type identification in van der Pauwâ€“Hall measurements. Applied Physics Letters, 2008, 93, .	3.3	85
158	Sources of unintentional conductivity in InN. Applied Physics Letters, 2008, 92, 032104.	3.3	85
159	First-principles calculations of diffusion coefficients: Hydrogen in silicon. Physical Review Letters, 1990, 64, 1401-1404.	7.8	84
160	Role of Si and Ge as impurities in ZnO. Physical Review B, 2009, 80, .	3.2	84
161	Reconstructions and origin of surface states on AlN polar and nonpolar surfaces. Physical Review B, 2009, 80, .	3.2	83
162	Structure, energetics, and vibrational properties of Si-H bond dissociation in silicon. Physical Review B, 1999, 59, 12884-12889.	3.2	82

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163	Magnesium incorporation in GaN grown by molecular-beam epitaxy. Applied Physics Letters, 2001, 78, 285-287.	3.3	82
164	BaSnO3 as a channel material in perovskite oxide heterostructures. Applied Physics Letters, 2016, 108, .	3.3	81
165	Correct Implementation of Polarization Constants in Wurtzite Materials and Impact on III-Nitrides. Physical Review X, 2016, 6, .	8.9	81
166	First-Principles Analysis of Radiative Recombination in Lead-Halide Perovskites. ACS Energy Letters, 2018, 3, 2329-2334.	17.4	81
167	Strain effects on the electronic structure of SrTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>: Toward high electron mobilities. Physical Review B, 2011, 84, .	3.2	79
168	Distribution of donor states on etched surface of AlGaN/GaN heterostructures. Journal of Applied Physics, 2010, 108, 063719.	2.5	78
169	Influence of microstructure on the carrier concentration of Mg-doped GaN films. Applied Physics Letters, 2001, 79, 2734-2736.	3.3	77
170	First-principles calculations of indirect Auger recombination in nitride semiconductors. Physical Review B, 2015, 92, .	3.2	77
171	First-principles analysis of electron transport in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaSnO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2017, 95, .	3.2	77
172	Carbon dimer defect as a source of the 4.1 eV luminescence in hexagonal boron nitride. Applied Physics Letters, 2019, 115, .	3.3	77
173	Structure, energetics, and dissociation of Si-H bonds at dangling bonds in silicon. Physical Review B, 1994, 49, 14766-14769.	3.2	76
174	Iodine interstitials as a cause of nonradiative recombination in hybrid perovskites. Physical Review B, 2020, 101, .	3.2	76
175	Atomic arrangement at the AlN/SiC interface. Physical Review B, 1996, 53, 7473-7478.	3.2	75
176	High optical polarization ratio from semipolar (202Â¯1Â¯) blue-green InGaN/GaN light-emitting diodes. Applied Physics Letters, 2011, 99, .	3.3	75
177	Controlling n-Type Doping in MoO₃. Chemistry of Materials, 2017, 29, 2563-2567.	6.7	74
178	Controlling the conductivity of InN. Physica Status Solidi (A) Applications and Materials Science, 2010, 207, 1024-1036.	1.8	72
179	Passivation and Doping due to Hydrogen in III-Nitrides. Physica Status Solidi (B): Basic Research, 2001, 228, 303-307.	1.5	71
180	Effects of an Electrically Conducting Layer at the Zinc Oxide Surface. Japanese Journal of Applied Physics, 2005, 44, 7271-7274.	1.5	71

#	Article	IF	Citations
181	Correctly Assessing Defect Tolerance in Halide Perovskites. Journal of Physical Chemistry C, 2020, 124, 6022-6027.	3.1	70
182	Dangling Bonds in Hexagonal Boron Nitride as Single-Photon Emitters. Physical Review Letters, 2019, 123, 127401.	7.8	68
183	Silicon-hydrogen bonding and hydrogen diffusion in amorphous silicon. Physical Review B, 1995, 51, 10615-10618.	3.2	67
184	Strain effects and band parameters in MgO, ZnO, and CdO. Applied Physics Letters, 2012, 101, .	3.3	67
185	Polycrystalline nitride semiconductor light-emitting diodes fabricated on quartz substrates. Applied Physics Letters, 2000, 76, 2182-2184.	3.3	66
186	Self-consistent band-gap corrections in density functional theory using modified pseudopotentials. Physical Review B, 2007, 75, .	3.2	66
187	Distributed surface donor states and the two-dimensional electron gas at AlGaN/GaN heterojunctions. Journal Physics D: Applied Physics, 2010, 43, 505501.	2.8	66
188	Defects in SiC for quantum computing. Journal of Applied Physics, 2011, 109, .	2.5	66
189	Advances in electronic structure methods for defects and impurities in solids. Physica Status Solidi (B): Basic Research, 2011, 248, 19-27.	1.5	66
190	Effects of strain on the electron effective mass in GaN and AlN. Applied Physics Letters, 2013, 102, .	3.3	66
191	Theory of Point Defects and Complexes in GaN. Materials Research Society Symposia Proceedings, 1995, 395, 645.	0.1	64
192	Determination of Internal Loss in Nitride Lasers from First Principles. Applied Physics Express, 2010, 3, 082101.	2.4	64
193	Structural origins of the properties of rare earth nickelate superlattices. Physical Review B, 2013, 87, .	3.2	64
194	Iron as a source of efficient Shockley-Read-Hall recombination in GaN. Applied Physics Letters, 2016, 109, .	3.3	64
195	Unexpectedly Strong Auger Recombination in Halide Perovskites. Advanced Energy Materials, 2018, 8, 1801027.	19.5	64
196	Hydrogen interactions with acceptor impurities in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SnO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms First-principles calculations. Physical Review B, 2009, 79, .	3.2	63
197	Structural identification of hydrogen and muonium centers in silicon: First-principles calculations of hyperfine parameters. Physical Review Letters, 1990, 64, 669-672.	7.8	62
198	Hydrogen as a shallow center in semiconductors and oxides. Physica Status Solidi (B): Basic Research, 2003, 235, 89-95.	1.5	62

#	Article	IF	Citations
199	Unusual Formation of Point-Defect Complexes in the Ultrawide-Band-Gap Semiconductor <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î²</mml:mi><mml:mtext>â^'</mml:mtext><mml:msub><mml:mrow><mml:mi>Ga</mml:mi></mml:mrow><mml:mrow><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review X, 2019, 9, .	3.2	62
200	Doping of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ga</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> with transition metals. Physical Review B, 2016, 94, .	3.2	61
201	Large and composition-dependent band gap bowing in InxGa1â^'xN alloys. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1999, 59, 274-278.	3.5	60
202	Effect of composition on the band gap of strained InxGa1â^'xN alloys. Journal of Applied Physics, 2003, 93, 4340-4342.	2.5	60
203	Indium versus hydrogen-terminated GaN(0001) surfaces: Surfactant effect of indium in a chemical vapor deposition environment. Applied Physics Letters, 2004, 84, 4322-4324.	3.3	60
204	Analysis of a conducting channel at the native zinc oxide surface. Superlattices and Microstructures, 2006, 39, 8-16.	3.1	60
205	Elastic Constants and Pressure-Induced Effects in MoS₂. Journal of Physical Chemistry C, 2014, 118, 12073-12076.	3.1	60
206	Arsenic impurities in GaN. Applied Physics Letters, 2000, 76, 1009-1011.	3.3	59
207	Room-temperature continuous-wave operation of InGaN multiple-quantum-well laser diodes with an asymmetric waveguide structure. Applied Physics Letters, 1999, 75, 581-583.	3.3	56
208	Band parameters and strain effects in ZnO and group-III nitrides. Semiconductor Science and Technology, 2011, 26, 014037.	2.0	56
209	Accurate and efficient band-offset calculations from density functional theory. Computational Materials Science, 2018, 151, 174-180.	3.0	56
210	Microscopic theory of hydrogen in silicon devices. IEEE Transactions on Electron Devices, 2000, 47, 1779-1786.	3.0	55
211	Identification of hydrogen configurations inp-type GaN through first-principles calculations of vibrational frequencies. Physical Review B, 2003, 68, .	3.2	55
212	Vacancy defects in indium oxide: An ab-initio study. Current Applied Physics, 2011, 11, S296-S300.	2.4	55
213	Effects of hole localization on limiting p-type conductivity in oxide and nitride semiconductors. Journal of Applied Physics, 2014, 115, 012014.	2.5	55
214	A first-principles understanding of point defects and impurities in GaN. Journal of Applied Physics, 2021, 129, .	2.5	55
215	Electronic structure of nitride surfaces. Journal of Crystal Growth, 2007, 300, 199-203.	1.5	54
216	First-principles study of the formation and migration of native defects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>NaAlH</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2009, 80, .	3.2	54

#	Article	IF	Citations
217	Influence of polarity on carrier transport in semipolar (2021Â¯) and (202Â¯1) multiple-quantum-well light-emitting diodes. Applied Physics Letters, 2012, 100, .	3.3	54
218	First-principles surface energies for monoclinic Ga2O3 and Al2O3 and consequences for cracking of (AlxGa1â^'x)2O3. APL Materials, 2020, 8, .	5.1	53
219	Group-V impurities in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SnO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> first-principles calculations. Physical Review B, 2010, 81, .	3.2	52
220	Dangling bonds and vacancies in germanium. Physical Review B, 2013, 87, .	3.2	52
221	Firstâ€Principles Simulation of Carrier Recombination Mechanisms in Halide Perovskites. Advanced Energy Materials, 2020, 10, 1902830.	19.5	52
222	Energetics of bond-centered hydrogen in strained Si-Si bonds. Physical Review B, 1995, 51, 2636-2639.	3.2	51
223	Limitations to the room temperature mobility of two- and three-dimensional electron liquids in SrTiO3. Applied Physics Letters, 2015, 106, .	3.3	51
224	Donor defects and small polarons on the TiO2(110) surface. Journal of Applied Physics, 2016, 119, .	2.5	51
225	Defect identification based on first-principles calculations for deep level transient spectroscopy. Applied Physics Letters, 2018, 113, .	3.3	51
226	Universal alignment of hydrogen levels in semiconductors and insulators. Physica B: Condensed Matter, 2006, 376-377, 1-6.	2.7	50
227	Hydrogen donors in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SnO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> by infrared spectroscopy and first-principles calculations. Physical Review B, 2010, 82, .	3.2	50
228	Defects in AlN as candidates for solid-state qubits. Physical Review B, 2016, 93, .	3.2	50
229	Electron and chemical reservoir corrections for point-defect formation energies. Physical Review B, 2016, 93, .	3.2	50
230	Three-Dimensional Spin Texture in Hybrid Perovskites and Its Impact on Optical Transitions. Journal of Physical Chemistry Letters, 2018, 9, 2903-2908.	4.6	50
231	Nonrad: Computing nonradiative capture coefficients from first principles. Computer Physics Communications, 2021, 267, 108056.	7.5	50
232	Effects of strain on the optical and vibrational properties of ZnSe-ZnSxSe1-x strained-layer superlattices. Journal of Luminescence, 1990, 46, 109-136.	3.1	48
233	Theoretical aspects of hydrogen in crystalline semiconductors. Physica B: Condensed Matter, 1991, 170, 21-32.	2.7	48
234	Formation and migration of charged native point defects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>MgH</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> First-principles calculations. Physical Review B, 2009, 80, .	3.2	48

#	Article	IF	Citations
235	Intrinsic and extrinsic causes of electron accumulation layers on InAs surfaces. Applied Physics Letters, 2010, 97, .	3.3	48
236	Electronic and protonic conduction in LaFeO₃. Journal of Materials Chemistry A, 2017, 5, 15367-15379.	10.3	48
237	Native defects and impurities in GaN. FestkÃ¶rperprobleme, 1996, , 25-44.	0.7	47
238	Band alignments and polarization properties of BN polymorphs. Applied Physics Express, 2014, 7, 031001.	2.4	46
239	First-principles study of the mobility of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2014, 90, .	3.2	45
240	First-principles study of van der Waals interactions in MoS₂and MoO₃. Journal of Physics Condensed Matter, 2014, 26, 305502.	1.8	45
241	Impact of Group-II Acceptors on the Electrical and Optical Properties of GaN. Japanese Journal of Applied Physics, 2013, 52, 08JJ04.	1.5	44
242	Quantum computing with defects. MRS Bulletin, 2013, 38, 802-807.	3.5	44
243	Sub-band-gap absorption in Ga2O3. Applied Physics Letters, 2017, 111, .	3.3	44
244	Hydrogen bonds in Al2O3 as dissipative two-level systems in superconducting qubits. Scientific Reports, 2014, 4, 7590.	3.3	43
245	Band discontinuities at heterojunctions between crystalline and amorphous silicon. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 1995, 13, 1635.	1.6	42
246	Phase separation in InGaN multiple quantum wells annealed at high nitrogen pressures. Applied Physics Letters, 1999, 75, 3950-3952.	3.3	42
247	Stretched-exponential relaxation modeled without invoking statistical distributions. Physical Review B, 1996, 53, 11292-11295.	3.2	41
248	Origins of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>n</mml:mi></mml:math> -type doping difficulties in perovskite stannates. Physical Review B, 2018, 97, .	3.2	41
249	Hybrid functional calculations of point defects and hydrogen in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">SrZrO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2014, 89, .	3.2	40
250	Hydrogen interactions with self-interstitials in silicon. Physical Review B, 1995, 52, R14320-R14323.	3.2	39
251	Structure and energetics of nitride surfaces under MOCVD growth conditions. Journal of Crystal Growth, 2003, 248, 8-13.	1.5	39
252	Surface Structures, Surfactants and Diffusion at Cubic and Wurtzite GaN. MRS Internet Journal of Nitride Semiconductor Research, 1998, 3, 1.	1.0	38

#	Article	IF	Citations
253	Performance and degradation of continuous-wave InGaN multiple-quantum-well laser diodes on epitaxially laterally overgrown GaN substrates. Applied Physics Letters, 2000, 77, 1931-1933.	3.3	38
254	Point defects in Al2O3 and their impact on gate stacks. Microelectronic Engineering, 2009, 86, 1756-1759.	2.4	38
255	Effect of transition-metal additives on hydrogen desorption kinetics of MgH2. Applied Physics Letters, 2013, 102, .	3.3	38
256	Doping of AlxGa1â^'xN alloys. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1999, 59, 253-257.	3.5	37
257	Stability, diffusivity, and vibrational properties of monatomic and molecular hydrogen in wurtzite GaN. Physical Review B, 2003, 68, .	3.2	37
258	A pathway to p-type wide-band-gap semiconductors. Applied Physics Letters, 2009, 95, .	3.3	37
259	Theoretical study of Schottky-barrier formation at epitaxial rare-earth-metal/semiconductor interfaces. Physical Review B, 2010, 81, .	3.2	37
260	Role of point defects in the electrical and optical properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>In</mml:mi><mml:mn>2</mml:mn></mml:m mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review Materials, 2019, 3, .	2.4	37
261	Hydrogenated vacancies and hidden hydrogen in SrTiO3. Physical Review B, 2014, 89, .	3.2	36
262	Lack of quantum confinement in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ga</mml:mi><mml:mn>2</mml:mn></mml:m mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> nanolayers. Physical Review B, 2017, 96, .	3.2	36
263	Hydrogen in silicon: Fundamental properties and consequences for devices. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1998, 16, 1767-1771.	2.1	35
264	Hydrogen-related defects and the role of metal additives in the kinetics of complex hydrides: A first-principles study. Physical Review B, 2009, 80, .	3.2	35
265	Insulating state of ultrathin epitaxial LaNiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>thin films detected by hard x-ray photoemission. Physical Review B, 2011, 84, .	3.2	35
266	Optical polarization characteristics of semipolar (303Â¯1) and (303Â¯1Â¯) InGaN/GaN light-emitting diodes. Optics Express, 2013, 21, A53.	3.4	35
267	First-principles study of vacancy-assisted impurity diffusion in ZnO. APL Materials, 2014, 2, 096101.	5.1	35
268	Structural investigation of the bilayer iridate<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Sr</mml:mi><mml:mn>3</mml:mn></mml:m mathvariant="normal">O</mml:mi><mml:mn>7</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2016, 93, .	3.2	35
269	Atomic scale investigation of aluminum incorporation, defects, and phase stability in Î²-(AlxGa1â^'x)2O3 films. APL Materials, 2021, 9, .	5.1	35
270	Defect tolerance in halide perovskites: A first-principles perspective. Journal of Applied Physics, 2022, 131, .	2.5	35

#	Article	IF	Citations
271	Strained-layer interfaces between IIâ€“VI compound semiconductors. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 1988, 6, 1350.	1.6	34
272	Role of strain in polarization switching in semipolar InGaN/GaN quantum wells. Applied Physics Letters, 2010, 97, 181102.	3.3	34
273	Free-carrier absorption in transparent conducting oxides: Phonon and impurity scattering in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SnO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml Physical Review B, 2015, 92, .	3.2	34
274	Linear Hyperfine Tuning of Donor Spins in Silicon Using Hydrostatic Strain. Physical Review Letters, 2018, 120, 167701.	7.8	34
275	Small polarons and point defects in barium cerate. Physical Review B, 2015, 92, .	3.2	33
276	Mechanism for the decomposition of lithium borohydride. International Journal of Hydrogen Energy, 2012, 37, 5825-5832.	7.1	32
277	Defects at Ge/oxide and IIIâ€“V/oxide interfaces. Microelectronic Engineering, 2013, 109, 211-215.	2.4	32
278	Hydrogen-induced metastable changes in the electrical conductivity of polycrystalline silicon. Physical Review Letters, 1994, 72, 3393-3396.	7.8	31
279	Role of hydrogen in surface reconstructions and growth of GaN. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 2002, 20, 1640.	1.6	31
280	Hybrid functional calculations of native point defects in InN. Physica Status Solidi (A) Applications and Materials Science, 2012, 209, 65-70.	1.8	31
281	Native point defects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>LaAlO</mml:mtext><mml:mn>3</mml:mn></mml:msub></mml:math> A hybrid functional study. Physical Review B, 2013, 88, .	3.2	31
282	Physics and chemistry of hydrogen in the vacancies of semiconductors. Physical Review B, 2003, 68, .	3.2	30
283	Auger Recombination in GaAs from First Principles. ACS Photonics, 2014, 1, 643-646.	6.6	30
284	Electrical and optical properties of iron in GaN, AlN, and InN. Physical Review B, 2019, 99, .	3.2	30
285	Native Defects and Impurities in Cubic and Wurtzite Gan. Materials Research Society Symposia Proceedings, 1994, 339, 687.	0.1	29
286	Doping of AlGaN Alloys. MRS Internet Journal of Nitride Semiconductor Research, 1999, 4, 890-901.	1.0	29
287	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, .	2.5	29
288	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, .	3.2	29

#	Article	IF	Citations
289	Posner molecules: from atomic structure to nuclear spins. Physical Chemistry Chemical Physics, 2018, 20, 12373-12380.	2.8	29
290	Doping limits in ZnSe. Physica B: Condensed Matter, 1993, 185, 118-127.	2.7	28
291	Exchange of deeply trapped and interstitial hydrogen in silicon. Physical Review B, 1999, 59, 5493-5497.	3.2	28
292	Ferroelastic switching of doped zirconia: Modeling and understanding from first principles. Physical Review B, 2014, 90, .	3.2	28
293	Effects of In profile on simulations of InGaN/GaN multi-quantum-well light-emitting diodes. Applied Physics Letters, 2014, 105, .	3.3	28
294	All-inorganic halide perovskites as candidates for efficient solar cells. Cell Reports Physical Science, 2021, 2, 100604.	5.6	28
295	Energetics and vibrational frequencies of interstitial H2 molecules in semiconductors. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1999, 58, 17-23.	3.5	27
296	Near-infrared absorption and semimetal-semiconductor transition in 2nm ErAs nanoparticles embedded in GaAs and AlAs. Applied Physics Letters, 2008, 92, .	3.3	27
297	Role of Atomic Multiplets in the Electronic Structure of Rare-Earth Semiconductors and Semimetals. Physical Review Letters, 2009, 102, 096401.	7.8	27
298	Mechanisms for the decomposition and dehydrogenation of Li amide/imide. Physical Review B, 2012, 85, .	3.2	27
299	Electronic structure of a single-layer InN quantum well in a GaN matrix. Applied Physics Letters, 2013, 102, .	3.3	27
300	Structural and electronic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrZrO</mml:mi><mml:mn>3</mml:mn></mml:msub></m Sr(Ti,Zr)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>alloys. Physical Review B, 2015, 92, .	3.2	27
301	Strain and the interpretation of band-lineup measurements. Physical Review Letters, 1987, 59, 946-946.	7.8	26
302	Entropy-Driven Stabilization of a Novel Configuration for Acceptor-Hydrogen Complexes in GaN. Physical Review Letters, 2001, 87, 205505.	7.8	26
303	Structure and energetics of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaAlO</mml:mi><mml:mn>3</mml:mn></mml:msub><m surfaces. Physical Review B, 2014, 90, .	3.2	26
304	Deep donor state of the copper acceptor as a source of green luminescence in ZnO. Applied Physics Letters, 2017, 111, 042101.	3.3	26
305	Impact of native defects in highâ€k dielectric oxides on GaN/oxide metalâ€“oxideâ€“semiconductor devices. Physica Status Solidi (B): Basic Research, 2013, 250, 787-791.	1.5	25
306	Turning<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></m a Mott insulator. Physical Review B, 2014, 90, .	3.2	25

#	Article	IF	Citations
307	Phase transformations upon doping in WO3. Journal of Chemical Physics, 2017, 146, 214504.	3.0	25
308	Optimizing Proton Conductivity in Zirconates through Defect Engineering. ACS Applied Energy Materials, 2019, 2, 2611-2619.	5.1	25
309	Band bowing and the direct-to-indirect crossover in random BAlN alloys. Physical Review Materials, 2017, 1, .	2.4	25
310	Step-flow growth of ZnO(0001) on GaN(0001) by metalorganic chemical vapor epitaxy. Journal of Crystal Growth, 2008, 310, 3407-3412.	1.5	24
311	Optimizing optical absorption of TiO2 by alloying with TiS2. Applied Physics Letters, 2008, 92, .	3.3	24
312	Ab initio study of enhanced thermal conductivity in ordered AlGaO3 alloys. Applied Physics Letters, 2019, 115, .	3.3	24
313	Orientation-dependent band offsets between (AlxGa1â^'x)2O3 and Ga2O3. Applied Physics Letters, 2020, 117, .	3.3	24
314	Vibrational and vibronic structure of isolated point defects: The nitrogen-vacancy center in diamond. Physical Review B, 2021, 104, .	3.2	24
315	Comment on â€˜â€˜Heterojunction valence-band-discontinuity dependence on face orientationâ€™â€™. Physical Review B, 1988, 37, 4801-4802.	3.2	23
316	Hydrogen in semiconductors and insulators. Journal of Alloys and Compounds, 2007, 446-447, 48-51.	5.5	23
317	Acceptor doping in the proton conductor SrZrO₃. Physical Chemistry Chemical Physics, 2017, 19, 11485-11491.	2.8	23
318	Computational studies of conductivity in wide-band-gap semiconductors and oxides. Journal of Physics Condensed Matter, 2008, 20, 064230.	1.8	22
319	Small hole polarons in rare-earth titanates. Applied Physics Letters, 2015, 106, .	3.3	22
320	Point defects, impurities, and small hole polarons in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">GdTiO</mml:mi></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2016, 93, .	3.2	22
321	Hybrid functional study of native point defects and impurities in ZnGeN2. Journal of Applied Physics, 2017, 122, .	2.5	22
322	Properties of In-Doped ZnO Films Grown by Metalorganic Chemical Vapor Deposition on GaN(0001) Templates. Journal of Electronic Materials, 2010, 39, 608-611.	2.2	21
323	Influence of Mg-doped barriers on semipolar (202Â¯1) multiple-quantum-well green light-emitting diodes. Applied Physics Letters, 2011, 99, 141114.	3.3	21
324	Interband and polaronic excitations in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>YTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> from first principles. Physical Review B, 2014, 90, .	3.2	21

#	Article	IF	Citations
325	Brittle fracture toughnesses of GaN and AlN from first-principles surface-energy calculations. Applied Physics Letters, 2015, 106, .	3.3	21
326	High optical power and lowâ€efficiency droop blue lightâ€emitting diodes using compositionally stepâ€graded InGaN barrier. Electronics Letters, 2015, 51, 1187-1189.	1.0	21
327	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.	3.0	21
328	Theory of Point Defects and Interfaces. Materials Research Society Symposia Proceedings, 1996, 449, 861.	0.1	20
329	Mutual Passivation of Electrically Active and Isovalent Impurities in Dilute Nitrides. Physical Review Letters, 2008, 100, 045505.	7.8	20
330	First-principles study of high-field-related electronic behavior of group-III nitrides. Physical Review B, 2014, 90, .	3.2	20
331	Characteristics of InGaN-AlGaN multiple-quantum-well laser diodes. IEEE Journal of Selected Topics in Quantum Electronics, 1998, 4, 498-504.	2.9	19
332	The Particleâ€Size Dependence of the Activation Energy for Decomposition of Lithium Amide. Angewandte Chemie - International Edition, 2011, 50, 10170-10173.	13.8	19
333	Decomposition mechanism and the effects of metal additives on the kinetics of lithium alanate. Physical Chemistry Chemical Physics, 2012, 14, 2840.	2.8	19
334	Calcium as a nonradiative recombination center in InGaN. Applied Physics Express, 2017, 10, 021001.	2.4	19
335	Band alignments and polarization properties of the Zn-IV-nitrides. Journal of Materials Chemistry C, 2020, 8, 7890-7898.	5.5	19
336	Nitrogen doping in ZnSe and ZnTe. Solid State Communications, 1995, 93, 447-450.	1.9	18
337	Theory of Hydrogen in GaN. Semiconductors and Semimetals, 1999, , 479-502.	0.7	18
338	Performance and optical gain characteristic of InGaN MQW laser diodes. Journal of Luminescence, 2000, 87-89, 135-139.	3.1	18
339	Hole polarons and p -type doping in boron nitride polymorphs. Physical Review B, 2017, 96, .	3.2	18
340	First-principles study of bandgap bowing in BGaN alloys. Journal of Applied Physics, 2019, 126, 095706.	2.5	18
341	Hidden role of Bi incorporation in nonradiative recombination in methylammonium lead iodide. Journal of Materials Chemistry A, 2020, 8, 12964-12967.	10.3	18
342	Spinning up quantum defects in 2D materials. Nature Materials, 2020, 19, 487-489.	27.5	18

#	Article	IF	Citations
343	Role of carbon and hydrogen in limiting <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>n</mml:mi></mml:math> -type doping of monoclinic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>(</mml:mo><mml:msub><mml:mi>Al</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi>O</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mo>)</mml:mo></mml:mrow></mml:math> ma. Physical Review B, 2022, 105, .	3.2	18
344	Band Offsets at Strained-Layer Interfaces. Materials Research Society Symposia Proceedings, 1987, 102, 565.	0.1	17
345	Identification of yellow luminescence centers in Be-doped GaN through pressure-dependent studies. Journal Physics D: Applied Physics, 2017, 50, 22LT03.	2.8	17
346	Strategies for p-type doping of ZnGeN2. Applied Physics Letters, 2019, 114, .	3.3	17
347	First-principles calculations of hyperfine interaction, binding energy, and quadrupole coupling for shallow donors in silicon. Npj Computational Materials, 2020, 6, .	8.7	17
348	Epitaxial ScxAl1â^'xN on GaN exhibits attractive high-K dielectric properties. Applied Physics Letters, 2022, 120, .	3.3	17
349	Electrical activity of hydrogen impurities in GaSb: First-principles calculations. Physical Review B, 2008, 78, .	3.2	16
350	Confinement effects on valence-subband character and polarization anisotropy in (112Â¯2) semipolar InGaN/GaN quantum wells. Journal of Applied Physics, 2012, 111, 073113.	2.5	16
351	First-principles study of surface charging in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>LaAlO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2015, 92, .	3.2	16
352	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, .	2.1	16
353	Anomalous Auger Recombination in PbSe. Physical Review Letters, 2020, 125, 037401.	7.8	16
354	Determination of the Mott-Hubbard gap inGdTiO3. Physical Review B, 2015, 92, .	3.2	15
355	Hydrogen intercalation in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> Physical Review B, 2016, 94, .	3.2	15
356	Ion-Transport Engineering of Alkaline-Earth Hydrides for Hydride Electrolyte Applications. Chemistry of Materials, 2018, 30, 5878-5885.	6.7	15
357	Giant polarization charge density at lattice-matched GaN/ScN interfaces. Applied Physics Letters, 2019, 115, .	3.3	15
358	Piezoelectric effect and polarization switching in Al1â^'xScxN. Journal of Applied Physics, 2021, 130, .	2.5	15
359	Band offsets at interfaces between HgTe, CdTe, and InSb. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 1987, 5, 1225.	1.6	14
360	Properties of hydrogen in crystalline silicon under compression and tension. Physical Review Letters, 1989, 63, 1090-1093.	7.8	14

#	Article	IF	Citations
361	Hydrogen in GaN. Materials Research Society Symposia Proceedings, 1995, 395, 723.	0.1	14
362	Electronic materials theory: Interfaces and defects. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2003, 21, S182-S190.	2.1	14
363	Role of hydrogen at germanium/dielectric interfaces. Thin Solid Films, 2008, 517, 144-147.	1.8	14
364	Effects of La 5d and 4f states on the electronic and optical properties of LaAlO3. Physical Review B, 2016, 94, .	3.2	14
365	First-principles study of direct and indirect optical absorption in BaSnO3. Applied Physics Letters, 2018, 112, 062106.	3.3	14
366	Limitations of In2O3 as a transparent conducting oxide. Applied Physics Letters, 2019, 115, .	3.3	14
367	Radiative capture rates at deep defects from electronic structure calculations. Physical Review B, 2020, 102, .	3.2	14
368	Finite-size correction for slab supercell calculations of materials with spontaneous polarization. Npj Computational Materials, 2021, 7, .	8.7	14
369	Spin-polarized calculations and hyperfine parameters for hydrogen or muonium in GaAs. Physical Review B, 1993, 47, 4256-4260.	3.2	13
370	Enhanced Optical Absorption Due to Symmetry Breaking in TiO_{2(1â€“x)}S_{2x} Alloys. Journal of Physical Chemistry C, 2013, 117, 4189-4193.	3.1	13
371	Deepâ€Level Defects and Impurities in InGaN Alloys. Physica Status Solidi (B): Basic Research, 2020, 257, 1900534.	1.5	13
372	First-principles study of electron transport in ScN. Physical Review B, 2021, 104, .	3.2	13
373	Atomic and electronic structure ofCaSi2/Si interfaces. Physical Review B, 1991, 43, 11913-11919.	3.2	12
374	Comment on "Electron Paramagnetic Resonance of Molecular Hydrogen in Silicon". Physical Review Letters, 1994, 73, 1456-1456.	7.8	12
375	Metalorganic chemical vapor deposition of ZnO(0001) thin films on GaN(0001) templates and ZnO(0001) substrates. Physica Status Solidi C: Current Topics in Solid State Physics, 2008, 5, 3091-3094.	0.8	12
376	Hydrogen Passivation of Impurities in Al₂O₃. ACS Applied Materials & Interfaces, 2014, 6, 4149-4153.	8.0	12
377	Sulfur doping of AlN and AlGaN for improved n-type conductivity. Physica Status Solidi - Rapid Research Letters, 2015, 9, 462-465.	2.4	12
378	Carbon-induced trapping levels in oxide dielectrics. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2015, 33, .	2.1	12

#	Article	IF	Citations
379	Conditions for T2 resistivity from electron-electron scattering. European Physical Journal B, 2017, 90, 1.	1.5	12
380	Role Of Hydrogen And Hydrogen Complexes In Doping Of Gan. Materials Research Society Symposia Proceedings, 1996, 423, 619.	0.1	11
381	Hydrogen in IIIâ€“V Nitrides. Semiconductors and Semimetals, 1999, , 157-184.	0.7	11
382	Theoretical study of the structural and electronic properties of strained ErAs. Physical Review B, 2008, 77, .	3.2	11
383	Vibrational signatures of OTe and OTeâ€“VCd in CdTe: A first-principles study. Computational Materials Science, 2010, 49, S242-S245.	3.0	11
384	Impact of Point Defects on Proton Conduction in Strontium Cerate. Journal of Physical Chemistry C, 2016, 120, 9562-9568.	3.1	11
385	Point-defect kinetics in Î±- and Î³-MgH2. International Journal of Hydrogen Energy, 2016, 41, 5688-5692.	7.1	11
386	Comment on â€œComparative study of ab initio nonradiative recombination rate calculations under different formalismsâ€• Physical Review B, 2018, 97, .	3.2	11
387	Phonon- and charged-impurity-assisted indirect free-carrier absorption in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Ga</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2019, 100, .	3.2	11
388	Role of Ga and In adatoms in the epitaxial growth of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î²</mml:mi><mml:mtext>â^'</mml:mtext><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2020, 102, .	3.2	11
389	Solubilities, defect reactions and doping limits in ZnSe. Journal of Crystal Growth, 1992, 117, 704-709.	1.5	10
390	Hydrogen-related defects in sodium alanate. Journal of Alloys and Compounds, 2007, 446-447, 459-461.	5.5	10
391	Dissipation-factor-based criterion for the validity of carrier-type identification by capacitance-voltage measurements. Applied Physics Letters, 2009, 94, 152110.	3.3	10
392	Alternative sources of p-type conduction in acceptor-doped ZnO. Applied Physics Letters, 2010, 97, 072112.	3.3	10
393	Impact of electric-field dependent dielectric constants on two-dimensional electron gases in complex oxides. Applied Physics Letters, 2015, 107, .	3.3	10
394	Interfacial Cation-Defect Charge Dipoles in Stacked TiO₂/Al₂O₃ Gate Dielectrics. ACS Applied Materials & Interfaces, 2018, 10, 5140-5146.	8.0	10
395	First-principles study of electron-phonon interactions and transport in anatase <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>TiO</mml:mi></mml:mrow><mml:mn>2</mml:mn> Physical Review B, 2019, 100, .	3.2	10
396	Hydrogen-Induced Degradation of NaMnO₂. Chemistry of Materials, 2019, 31, 5224-5228.	6.7	10

#	Article	IF	Citations
397	Electronic structure and magneto-optical properties of silicon-nitrogen-vacancy complexes in diamond. Physical Review B, 2020, 102, .	3.2	10
398	Thermodynamics of boron incorporation in BGaN. Physical Review Materials, 2021, 5, .	2.4	10
399	Mg doping and diffusion in (010) Î²-Ga2O3 films grown by plasma-assisted molecular beam epitaxy. Journal of Applied Physics, 2021, 130, .	2.5	10
400	Hydrogen states in silicon. Journal of Non-Crystalline Solids, 1998, 227-230, 111-119.	3.1	9
401	Effect of Si doping on the strain and defect structure of GaN thin films. Physica B: Condensed Matter, 1999, 273-274, 50-53.	2.7	9
402	Design and performance of asymmetric waveguide nitride laser diodes. IEEE Journal of Quantum Electronics, 2000, 36, 184-191.	1.9	9
403	Band gap changes of GaN shocked to 13 GPa. Applied Physics Letters, 2002, 80, 1912-1914.	3.3	9
404	Carbon-nitrogen molecules in GaAs and GaP. Physical Review B, 2008, 77, .	3.2	9
405	Polarization effects due to thickness fluctuations in nonpolar InGaN/GaN quantum wells. Applied Physics Letters, 2013, 103, 073115.	3.3	9
406	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.	3.3	9
407	Impact of nitrogen and carbon on defect equilibrium in ZrO2. Acta Materialia, 2016, 117, 286-292.	7.9	9
408	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	9
409	Carrier-induced absorption as a mechanism for electrochromism in tungsten trioxide. MRS Communications, 2018, 8, 926-931.	1.8	9
410	First-principles study of antisite defects in perovskite stannates. Journal of Applied Physics, 2019, 126, 195701.	2.5	9
411	Prospects for n-type conductivity in cubic boron nitride. Applied Physics Letters, 2021, 119, .	3.3	9
412	Chapter 16 Theory of Isolated Interstitial Hydrogen and Muonium in Crystalline Semiconductors. Semiconductors and Semimetals, 1991, 34, 585-622.	0.7	8
413	Theory of defects, impurities, and doping in ZnSe. Journal of Luminescence, 1992, 52, 1-8.	3.1	8
414	Defects and Doping in III-V Nitrides. Materials Science Forum, 1997, 258-263, 19-26.	0.3	8

#	Article	IF	Citations
415	DX CENTERS IN AlGaN. International Journal of Modern Physics B, 1999, 13, 1363-1378.	2.0	8
416	Theory of Hydrogen Interactions with Amorphous Silicon. Materials Research Society Symposia Proceedings, 1999, 557, 275.	0.1	8
417	Technology development & design for 22 nm InGaAs/InP-channel MOSFETs. , 2008, , .		8
418	Point-defect-mediated dehydrogenation of AlH3. Applied Physics Letters, 2010, 97, .	3.3	8
419	Effects of surface reconstructions on oxygen adsorption at AlN polar surfaces. Europhysics Letters, 2010, 89, 56004.	2.0	8
420	Controlling the Conductivity in Oxide Semiconductors. Springer Series in Materials Science, 2012, , 23-35.	0.6	8
421	Theory and Modeling of Oxide Semiconductors. Semiconductors and Semimetals, 2013, 88, 1-37.	0.7	8
422	Nitride-based high-electron-mobility transistor with single-layer InN for mobility-enhanced channel. Applied Physics Express, 2015, 8, 024302.	2.4	8
423	Electrical compensation mechanism in fluorine-doped SnO2. Applied Physics Letters, 2017, 111, .	3.3	8
424	Optimizing <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>n</mml:mi></mml:math> -type doping of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ZnGeN</mml:mi><mml:mn>2</mml:mn></mml:msub></ and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ZnSiN</mml:mi><mml:mn>2</mml:mn></mml:msub></m	3.2	8
425	Native Defect Compensation in Wide-Band-Gap Semiconductors. Materials Science Forum, 1992, 83-87, 1225-1234.	0.3	7
426	Atomic Hydrogen in GaN. Materials Research Society Symposia Proceedings, 1995, 378, 503.	0.1	7
427	Stability and mobility of native point defects in AlH3. Journal of Alloys and Compounds, 2011, 509, S658-S661.	5.5	7
428	Overcoming Bipolar Doping Difficulty in Wide Gap Semiconductors. , 2011, , 213-239.		7
429	LiH as a Li+ and Hâ¯ ion provider. Solid State Ionics, 2013, 253, 53-56.	2.7	7
430	Surprising stability of neutral interstitial hydrogen in diamond and cubic BN. Journal of Physics Condensed Matter, 2016, 28, 06LT01.	1.8	7
431	Identification of Microscopic Hole-Trapping Mechanisms in Nitride Semiconductors. IEEE Electron Device Letters, 2016, 37, 154-156.	3.9	7
432	Boron dangling bonds in a monolayer of hexagonal boron nitride. Journal of Applied Physics, 2021, 129, .	2.5	7

#	Article	IF	Citations
433	Adsorption and Diffusion of Aluminum on Î²-Ga₂O₃(010) Surfaces. ACS Applied Materials & Interfaces, 2021, 13, 10650-10655.	8.0	7
434	Incorporation of Si and Sn donors in Î²-Ga2O3 through surface reconstructions. Journal of Applied Physics, 2021, 130, 185703.	2.5	7
435	Hydrogen Diffusion and Passivation of Shallow Impurities in Crystalline Silicon. Materials Science Forum, 1989, 38-41, 979-984.	0.3	6
436	Silicon-Hydrogen Bonding and Hydrogen Diffusion in Amorphous Silicon. Materials Research Society Symposia Proceedings, 1995, 377, 389.	0.1	6
437	Theory of Hydrogen in Semiconductors. Materials Research Society Symposia Proceedings, 1998, 513, 55.	0.1	6
438	Physics of defects and hydrogen in dilute nitrides. IEE Proceedings: Optoelectronics, 2004, 151, 369-377.	0.8	6
439	First-principles investigations of F and Cl impurities in NaAlH4. Journal of Alloys and Compounds, 2009, 484, 347-351.	5.5	6
440	The role of native defects in the transport of charge and mass and the decomposition of Li₄BN₃H₁₀. Physical Chemistry Chemical Physics, 2014, 16, 25314-25320.	2.8	6
441	Band alignments between SmTiO3, GdTiO3, and SrTiO3. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2016, 34, .	2.1	6
442	Impact of dangling bonds on properties of h-BN. 2D Materials, 2021, 8, 024002.	4.4	6
443	Hydride Conductivity in Nitride Hydrides. ACS Applied Energy Materials, 2021, 4, 6348-6355.	5.1	6
444	Materials and device simulations for silicon qubit design and optimization. MRS Bulletin, 2021, 46, 634-641.	3.5	6
445	Summary Abstract: Theoretical investigations of fluorineâ€“silicon systems. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1988, 6, 1973-1974.	2.1	5
446	Atomic and Electronic Structure of Si-Ge Superlattices. Physical Review Letters, 1989, 62, 974-974.	7.8	5
447	Tight-Binding Initialization for Generating High-Quality Initial Wave Functions: Application to Defects and Impurities in GaN. Materials Research Society Symposia Proceedings, 1995, 408, 43.	0.1	5
448	Johnson, Herring, and Van de Walle Reply:. Physical Review Letters, 1995, 74, 4566-4566.	7.8	5
449	Inverted Order of Acceptor and Donor Levels of Monatomic Hydrogen in Silicon. Physical Review Letters, 1995, 74, 1889-1889.	7.8	5
450	Doping of Aigan Alloys. Materials Research Society Symposia Proceedings, 1998, 537, 1.	0.1	5

#	Article	IF	Citations
451	CW Operation of InGaN MQW Laser Diodes. Physica Status Solidi A, 2000, 180, 139-147.	1.7	5
452	Band alignment at bandâ€insulator/Mottâ€insulator interfaces. Physica Status Solidi - Rapid Research Letters, 2014, 8, 577-582.	2.4	5
453	Prospects for high carrier mobility in the cubic germanates. Semiconductor Science and Technology, 2020, 35, 085030.	2.0	5
454	Theoretical Study of Semiconductor Interfaces. Materials Research Society Symposia Proceedings, 1985, 63, 21.	0.1	4
455	Theoretical Study of Native Point Defects in Aln and InN. Materials Research Society Symposia Proceedings, 1997, 482, 910.	0.1	4
456	Effects of N on the electronic structures of H defects in IIIâ€“V semiconductors. Optical Materials, 2004, 25, 261-269.	3.6	4
457	Atomic and electronic structure of hydrogen-related centers in hydrogen storage materials. Physica B: Condensed Matter, 2009, 404, 793-797.	2.7	4
458	Multilayer transition-metal dichalcogenide channel Thin-Film Transistors. , 2012, , .		4
459	Polarization properties at rocksalt/wurtzite oxide interfaces. Physical Review B, 2020, 102, .	3.2	4
460	Structural, electronic, and polarization properties of YN and LaN. Physical Review Materials, 2021, 5, .	2.4	4
461	Fluorine-Silicon Reactions and the Etching of Crystalline Silicon. Materials Research Society Symposia Proceedings, 1988, 141, 425.	0.1	3
462	Phase Stability and Electronic Structure of GaAs_{1â€“x}N_x Alloys. Materials Research Society Symposia Proceedings, 1995, 379, 3.	0.1	3
463	Isolated Monatomic Hydrogen in Silicon. Semiconductors and Semimetals, 1999, 61, 13-23.	0.7	3
464	Hydrogen Interactions with Polycrystalline and Amorphous Siliconâ€”Theory. Semiconductors and Semimetals, 1999, 61, 241-281.	0.7	3
465	Theory of Impurities and Defects in III-Nitrides: Vacancies in GaN and Related Materials. Materials Science Forum, 2000, 338-342, 1561-1566.	0.3	3
466	Effects of Ionicity on Defect Physics of Wide-Band-Gap Semiconductors. Materials Science Forum, 2004, 457-460, 15-20.	0.3	3
467	Growth of In-doped ZnO films by metalorganic chemical vapor deposition on GaN(0001) templates. Physica Status Solidi C: Current Topics in Solid State Physics, 2009, 6, 1464-1467.	0.8	3
468	Homoepitaxial growth and characterization of ZnO(0001) thin films grown by metalorganic chemical vapor epitaxy. Physica Status Solidi C: Current Topics in Solid State Physics, 2009, 6, 1460-1463.	0.8	3

#	Article	IF	Citations
469	Hydrogen in oxides and nitrides: unexpected physics and impact on devices. IOP Conference Series: Materials Science and Engineering, 2010, 15, 012001.	0.6	3
470	Dehydrogenation of AlH₃ via the Vacancy Clustering Mechanism. Journal of Physical Chemistry C, 2012, 116, 12995-13002.	3.1	3
471	Effects of biaxial stress and layer thickness on octahedral tilts in LaNiO3. Applied Physics Letters, 2015, 107, 261901.	3.3	3
472	Sr3Ir2O7F2 : Topochemical conversion of a relativistic Mott state into a spin-orbit driven band insulator. Physical Review B, 2018, 98, .	3.2	3
473	Electron doping in Sr3Ir2O7 : Collapse of band gap and magnetic order. Physical Review B, 2018, 98, .	3.2	3
474	Inflection points in the conduction-band structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>BaSn</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2020, 102, .	3.2	3
475	Defect Chemistry and Hydrogen Transport in La/Sr-Based Oxyhydrides. Journal of Physical Chemistry C, 2021, 125, 2250-2256.	3.1	3
476	Understanding carbon contamination in the proton-conducting zirconates and cerates. Physical Chemistry Chemical Physics, 2021, 23, 14205-14211.	2.8	3
477	Hole Trapping at Acceptor Impurities and Alloying Elements in AlN. Physica Status Solidi - Rapid Research Letters, 2021, 15, 2100218.	2.4	3
478	Theory of Defects in Wide-Band-Gap Semiconductors. Materials Research Society Symposia Proceedings, 1995, 378, 467.	0.1	2
479	sComment on ``Surface silicon-deuterium bond energy from gas-phase equilibration''. Physical Review B, 1997, 55, 13314-13318.	3.2	2
480	MOCVD growth and characterization of AlGaInN multiple quantum well heterostructures and laser diodes. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1999, 59, 33-38.	3.5	2
481	Quantitative Analysis of Absorption and Field-Induced Absorption Changes in InGaN/GaN Quantum Wells. Physica Status Solidi (B): Basic Research, 2002, 234, 742-745.	1.5	2
482	Hydrogen Interactions With Semiconductors And Oxides. AIP Conference Proceedings, 2003, , .	0.4	2
483	Properties of ZnO(0001) layers grown by metalorganic chemical vapor deposition on GaN(0001) templates. Physica Status Solidi C: Current Topics in Solid State Physics, 2008, 5, 1733-1735.	0.8	2
484	Advanced Calculations for Defects in Solids â€“ Electronic Structure Methods. Physica Status Solidi (B): Basic Research, 2011, 248, 17-18.	1.5	2
485	Electrically active Er doping in InAs, In0.53Ga0.47As, and GaAs. Applied Physics Letters, 2012, 101, .	3.3	2
486	Conductivity and transparency of TiO2from first principles. , 2013, , .		2

#	Article	IF	Citations
487	Metal versus insulator behavior in ultrathin<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>-based heterostructures. Physical Review B, 2016, 94, .	3.2	2
488	Publisher's Note: Hole polarons and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>p</mml:mi></mml:math> -type doping in boron nitride polymorphs [Phys. Rev. B 96 , 100102(R) (2017)]. Physical Review B, 2018, 97, .	3.2	2
489	Impact of phonons and spin-orbit coupling on Auger recombination in InAs. Physical Review B, 2019, 100, .	3.2	2
490	First-principles study of transport in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>WO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml Physical Review B, 2020, 101, .	3.2	2
491	Defects and Impurities in Semiconductors. , 2005, , 1877-1888.		2
492	Theoretical study of band offsets at semiconductor interfaces. Perspectives in Condensed Matter Physics, 1988, , 268-279.	0.1	2
493	Anisotropic-strain-enhanced hole mobility in GaN by lattice matching to ZnGeN2 and MgSiN2. Applied Physics Letters, 2022, 120, .	3.3	2
494	First-Principles Investigations of Hydrogen and Fluorine on Silicon Surfaces. Materials Research Society Symposia Proceedings, 1992, 259, 375.	0.1	1
495	New Model for â€œStretched Exponentialâ€•Relaxation. Materials Research Society Symposia Proceedings, 1996, 420, 533.	0.1	1
496	Evidence for Oxygen DX Centers in AlGaN. Materials Research Society Symposia Proceedings, 1998, 512, 531.	0.1	1
497	Room-Temperature Continuous-Wave Operation of InGaN Multiple Quantum Well Laser Diodes with an Asymmetric Waveguide Structure. Physica Status Solidi A, 1999, 176, 49-52.	1.7	1
498	Performance characteristics of cw InGaN multiple-quantum-well laser diodes. Materials Research Society Symposia Proceedings, 2000, 639, 1061.	0.1	1
499	Stability, diffusion, and complex formation of beryllium in wurtzite GaN. Materials Research Society Symposia Proceedings, 2000, 639, 431.	0.1	1
500	Nanomembrane β-Ga<inf>2</inf>O<inf>3</inf> high-voltage field effect transistors. , 2013, , .		1
501	Auger recombination in InAs: Role of spin-orbit coupling and phonons. , 2016, , .		1
502	Ab initio study of hydrogenic effective mass impurities in Si nanowires. Journal of Physics Condensed Matter, 2017, 29, 095303.	1.8	1
503	First-principles calculations of optical transitions at native defects and impurities in ZnO. , 2018, , .		1
504	Impact of point defects on electrochromism in WO3. , 2018, , .		1

#	Article	IF	Citations
505	Surprising stability of polar (001) surfaces of the Mott insulator GdTiO3. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2021, 39, .	2.1	1
506	Theory of Hydrogen Reactions in Silicon. Materials Research Society Symposia Proceedings, 1987, 104, 253.	0.1	0
507	Pseudopotential Pseudocredit. Physics Today, 1987, 40, 124-124.	0.3	0
508	Enhanced and Retarded Diffusion of Shallow Impurities in Silicon. Materials Research Society Symposia Proceedings, 1988, 141, 243.	0.1	0
509	Atomic Structure of CaSi2/Si Interfaces. Materials Research Society Symposia Proceedings, 1989, 159, 115.	0.1	0
510	Electronic Structure and Hyperfine Parameters for Hydrogen and Muonium in Silicon. Materials Research Society Symposia Proceedings, 1989, 163, 419.	0.1	0
511	Self-Compensation and Doping Problems in ZnSe. Materials Research Society Symposia Proceedings, 1992, 242, 311.	0.1	0
512	First-Principles Investigations of Acceptors in ZnSe. Materials Research Society Symposia Proceedings, 1992, 242, 349.	0.1	0
513	Defects, doping, and interfaces in III-V nitrides. , 1998, , .		0
514	Novel conguration of Mg-H complexes in GaN. Materials Research Society Symposia Proceedings, 2001, 693, 339.	0.1	0
515	Auger recombination in light-emitting materials. , 2014, , .		0
516	Publisher's Note: Defects in AlN as candidates for solid-state qubits [Phys. Rev. B 93 , 161201(R) (2016)]. Physical Review B, 2018, 97, .	3.2	0
517	Controlling the conductivity of wide-band-gap semiconductors. Springer Proceedings in Physics, 2001, , 3-8.	0.2	0
518	Theoretical aspects of hydrogen in crystalline semiconductors. , 1991, , 21-32.		0
519	Doping limits in ZnSe. , 1993, , 118-127.		0
520	Publisher's Note: Band bowing and the direct-to-indirect crossover in random BAlN alloys [Phys. Rev. Materials 1 , 065001 (2017)]. Physical Review Materials, 2018, 2, .	2.4	0
521	First-Principles Calculations 1. Springer Series in Materials Science, 2020, , 309-328.	0.6	0
522	First-principles studies of diffusion in gallium oxide. , 2022, , .		0