

# Stephan Lany

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

160  
papers

12,030  
citations

58  
h-index

107  
g-index

171  
ext. papers

13,428  
ext. citations

6.8  
avg. IF

6.86  
L-index

#	Paper	IF	Citations
160	Bandgap analysis and carrier localization in cation-disordered ZnGeN <sub>2</sub> . <i>APL Materials</i> , <b>2022</b> , 10, 011112	5.7	1
159	Short-Range Order Tunes Optical Properties in Long-Range Disordered ZnSnN <sub>2</sub> /ZnO Alloy. <i>Chemistry of Materials</i> , <b>2022</b> , 34, 3910-3919	9.6	1
158	Computational discovery of stable and metastable ternary oxynitrides. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 234706	3.9	7
157	Computational Fermi level engineering and doping-type conversion of Mg:Ga <sub>2</sub> O <sub>3</sub> via three-step synthesis process. <i>Journal of Applied Physics</i> , <b>2021</b> , 129, 245704	2.5	2
156	Metal chalcogenides for neuromorphic computing: emerging materials and mechanisms. <i>Nanotechnology</i> , <b>2021</b> , 32,	3.4	6
155	Probing configurational disorder in ZnGeN <sub>2</sub> using cluster-based Monte Carlo. <i>Physical Review Materials</i> , <b>2021</b> , 5,	3.2	10
154	Combinatorial investigation of structural and optical properties of cation-disordered ZnGeN <sub>2</sub> . <i>Journal of Materials Chemistry C</i> , <b>2020</b> , 8, 8736-8746	7.1	11
153	Wurtzite materials in alloys of rock salt compounds. <i>Journal of Materials Research</i> , <b>2020</b> , 35, 972-980	2.5	0
152	Utilizing Site Disorder in the Development of New Energy-Relevant Semiconductors. <i>ACS Energy Letters</i> , <b>2020</b> , 5, 2027-2041	20.1	24
151	Templated Growth of Metastable Polymorphs on Amorphous Substrates with Seed Layers. <i>Physical Review Applied</i> , <b>2020</b> , 13,	4.3	3
150	Perfect short-range ordered alloy with line-compound-like properties in the ZnSnN <sub>2</sub> :ZnO system. <i>Npj Computational Materials</i> , <b>2020</b> , 6,	10.9	8
149	Combinatorial Synthesis of Magnesium Tin Nitride Semiconductors. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 8421-8430	16.4	19
148	Thin Film Synthesis of Semiconductors in the Mg <sub>3</sub> B <sub>2</sub> N <sub>3</sub> Materials System. <i>Chemistry of Materials</i> , <b>2019</b> , 31, 8717-8724	9.6	16
147	Interplay between Composition, Electronic Structure, Disorder, and Doping due to Dual Sublattice Mixing in Nonequilibrium Synthesis of ZnSnN <sub>2</sub> :O. <i>Advanced Materials</i> , <b>2019</b> , 31, e1807406	24	27
146	The role of decomposition reactions in assessing first-principles predictions of solid stability. <i>Npj Computational Materials</i> , <b>2019</b> , 5,	10.9	32
145	A map of the inorganic ternary metal nitrides. <i>Nature Materials</i> , <b>2019</b> , 18, 732-739	27	148
144	High-Throughput Experimental Study of Wurtzite Mn Zn O Alloys for Water Splitting Applications. <i>ACS Omega</i> , <b>2019</b> , 4, 7436-7447	3.9	4

143	Zn <sub>2</sub> SbN <sub>3</sub> : growth and characterization of a metastable photoactive semiconductor. <i>Materials Horizons</i> , <b>2019</b> , 6, 1669-1674	14.4	13
142	Computational Materials Design: Interplay between Composition, Electronic Structure, Disorder, and Doping due to Dual Sublattice Mixing in Nonequilibrium Synthesis of ZnSnN <sub>2</sub> O (Adv. Mater. 11/2019). <i>Advanced Materials</i> , <b>2019</b> , 31, 1970080	24	0
141	Predicting synthesizability. <i>Journal Physics D: Applied Physics</i> , <b>2019</b> , 52,	3	161
140	Electron scattering mechanisms in polycrystalline sputtered zinc tin oxynitride thin films. <i>Journal of Applied Physics</i> , <b>2019</b> , 126, 035701	2.5	12
139	Ternary nitride semiconductors in the rocksalt crystal structure. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2019</b> , 116, 14829-14834	11.5	31
138	Redox-Mediated Stabilization in Zinc Molybdenum Nitrides. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 4293-4301	16.4	34
137	Negative-pressure polymorphs made by heterostructural alloying. <i>Science Advances</i> , <b>2018</b> , 4, eaaq1442	14.3	25
136	Defect phase diagram for doping of Ga <sub>2</sub> O <sub>3</sub> . <i>APL Materials</i> , <b>2018</b> , 6, 046103	5.7	65
135	Communication: The electronic entropy of charged defect formation and its impact on thermochemical redox cycles. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 071101	3.9	13
134	Zn <sub>x</sub> Mn <sub>1-x</sub> O Solid Solutions in the Rocksalt Structure: Optical, Charge Transport, and Photoelectrochemical Properties. <i>ACS Applied Energy Materials</i> , <b>2018</b> , 1, 260-266	6.1	6
133	Band Edge Positions and Their Impact on the Simulated Device Performance of ZnSnN <sub>2</sub> -Based Solar Cells. <i>IEEE Journal of Photovoltaics</i> , <b>2018</b> , 8, 110-117	3.7	16
132	Zinc-Stabilized Manganese Telluride with Wurtzite Crystal Structure. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 18769-18775	3.8	9
131	Spin-orbit coupling effects on predicting defect properties with hybrid functionals: A case study in CdTe. <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	15
130	Semiconducting cubic titanium nitride in the Th <sub>3</sub> P <sub>4</sub> structure. <i>Physical Review Materials</i> , <b>2018</b> , 2,	3.2	17
129	Physical descriptor for the Gibbs energy of inorganic crystalline solids and temperature-dependent materials chemistry. <i>Nature Communications</i> , <b>2018</b> , 9, 4168	17.4	80
128	Electron Doping of Proposed Kagome Quantum Spin Liquid Produces Localized States in the Band Gap. <i>Physical Review Letters</i> , <b>2018</b> , 121, 186402	7.4	17
127	Exciton photoluminescence and benign defect complex formation in zinc tin nitride. <i>Materials Horizons</i> , <b>2018</b> , 5, 823-830	14.4	29
126	Perovskite-Inspired Photovoltaic Materials: Toward Best Practices in Materials Characterization and Calculations. <i>Chemistry of Materials</i> , <b>2017</b> , 29, 1964-1988	9.6	87

125	A computational framework for automation of point defect calculations. <i>Computational Materials Science</i> , <b>2017</b> , 130, 1-9	3.2	83
124	Trade-Offs in Thin Film Solar Cells with Layered Chalcostibite Photovoltaic Absorbers. <i>Advanced Energy Materials</i> , <b>2017</b> , 7, 1601935	21.8	35
123	Conduction band position tuning and Ga-doping in (Cd,Zn)S alloy thin films. <i>Materials Chemistry Frontiers</i> , <b>2017</b> , 1, 1342-1348	7.8	5
122	Solubility limits in quaternary SnTe-based alloys. <i>RSC Advances</i> , <b>2017</b> , 7, 24747-24753	3.7	12
121	Novel phase diagram behavior and materials design in heterostructural semiconductor alloys. <i>Science Advances</i> , <b>2017</b> , 3, e1700270	14.3	37
120	Optically induced metastability in Cu(In,Ga)Se. <i>Scientific Reports</i> , <b>2017</b> , 7, 13788	4.9	13
119	Selection Metric for Photovoltaic Materials Screening Based on Detailed-Balance Analysis. <i>Physical Review Applied</i> , <b>2017</b> , 8,	4.3	41
118	Characterization of defects in copper antimony disulfide. <i>Journal of Materials Chemistry A</i> , <b>2017</b> , 5, 21986-21993	6.3	33
117	Using heterostructural alloying to tune the structure and properties of the thermoelectric Sn <sub>1-x</sub> CaxSe. <i>Journal of Materials Chemistry A</i> , <b>2017</b> , 5, 16873-16882	13	16
116	Thermodynamic Routes to Novel Metastable Nitrogen-Rich Nitrides. <i>Chemistry of Materials</i> , <b>2017</b> , 29, 6936-6946	9.6	78
115	Computationally Driven Two-Dimensional Materials Design: What Is Next?. <i>ACS Nano</i> , <b>2017</b> , 11, 7560-7566	16.7	32
114	Design of Metastable Tin Titanium Nitride Semiconductor Alloys. <i>Chemistry of Materials</i> , <b>2017</b> , 29, 6511-6517	6.1	19
113	Monte Carlo simulations of disorder in ZnSnN <sub>2</sub> and the effects on the electronic structure. <i>Physical Review Materials</i> , <b>2017</b> , 1,	3.2	57
112	The effect of sub-oxide phases on the transparency of tin-doped gallium oxide. <i>Applied Physics Letters</i> , <b>2016</b> , 109, 141909	3.4	8
111	Accelerated development of CuSbS <sub>2</sub> thin film photovoltaic device prototypes. <i>Progress in Photovoltaics: Research and Applications</i> , <b>2016</b> , 24, 929-939	6.8	61
110	Roadmap on optical energy conversion. <i>Journal of Optics (United Kingdom)</i> , <b>2016</b> , 18, 073004	1.7	69
109	Revisiting the Valence and Conduction Band Size Dependence of PbS Quantum Dot Thin Films. <i>ACS Nano</i> , <b>2016</b> , 10, 3302-11	16.7	89
108	Wild band edges: The role of bandgap grading and band-edge fluctuations in high-efficiency chalcogenide devices <b>2016</b> ,		10

107	A review of defects and disorder in multinary tetrahedrally bonded semiconductors. <i>Semiconductor Science and Technology</i> , <b>2016</b> , 31, 123004	1.8	56
106	Electronic structures of Cu <sub>2</sub> O, Cu <sub>4</sub> O <sub>3</sub> , and CuO: A joint experimental and theoretical study. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	130
105	Synthesis of a mixed-valent tin nitride and considerations of its possible crystal structures. <i>Journal of Chemical Physics</i> , <b>2016</b> , 144, 144201	3.9	23
104	Understanding and Control of Bipolar Self-Doping in Copper Nitride. <i>Journal of Applied Physics</i> , <b>2016</b> , 119,	2.5	21
103	Pathway to oxide photovoltaics via band-structure engineering of SnO. <i>APL Materials</i> , <b>2016</b> , 4, 106103	5.7	23
102	Synthesis and Characterization of (Sn,Zn)O Alloys. <i>Chemistry of Materials</i> , <b>2016</b> , 28, 7765-7772	9.6	15
101	Semiconducting properties of spinel tin nitride and other IV <sub>3</sub> N <sub>4</sub> polymorphs. <i>Journal of Materials Chemistry C</i> , <b>2015</b> , 3, 1389-1396	7.1	40
100	Non-equilibrium synthesis, structure, and opto-electronic properties of Cu <sub>2</sub> x Zn x O alloys. <i>Journal of Materials Science</i> , <b>2015</b> , 50, 1350-1357	4.3	16
99	Design of Semiconducting Tetrahedral Mn <sub>1-x</sub> Zn <sub>x</sub> O Alloys and Their Application to Solar Water Splitting. <i>Physical Review X</i> , <b>2015</b> , 5,	9.1	30
98	Effect of extended strain fields on point defect phonon scattering in thermoelectric materials. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 19410-23	3.6	48
97	Semiconducting transition metal oxides. <i>Journal of Physics Condensed Matter</i> , <b>2015</b> , 27, 283203	1.8	111
96	Non-equilibrium alloying controls optoelectronic properties in Cu <sub>2</sub> O thin films for photovoltaic absorber applications. <i>Applied Physics Letters</i> , <b>2015</b> , 106, 123903	3.4	21
95	Self-regulated growth and tunable properties of CuSb <sub>2</sub> S <sub>2</sub> solar absorbers. <i>Solar Energy Materials and Solar Cells</i> , <b>2015</b> , 132, 499-506	6.4	97
94	Entropy-Driven Clustering in Tetrahedrally Bonded Multinary Materials. <i>Physical Review Applied</i> , <b>2015</b> , 3,	4.3	57
93	Effects of Disorder on Carrier Transport in Cu <sub>2</sub> SnS <sub>3</sub> . <i>Physical Review Applied</i> , <b>2015</b> , 4,	4.3	63
92	Extended antisite defects in tetrahedrally bonded semiconductors. <i>Physical Review B</i> , <b>2015</b> , 92,	3.3	16
91	CuSbSe <sub>2</sub> photovoltaic devices with 3% efficiency. <i>Applied Physics Express</i> , <b>2015</b> , 8, 082301	2.4	67
90	Structural and electronic modification of photovoltaic SnS by alloying. <i>Journal of Applied Physics</i> , <b>2014</b> , 115, 113507	2.5	27

89	Control of the Electrical Properties in Spinel Oxides by Manipulating the Cation Disorder. <i>Advanced Functional Materials</i> , <b>2014</b> , 24, 610-618	15.6	86
88	Enhanced Electron Mobility Due to Dopant-Defect Pairing in Conductive ZnMgO. <i>Advanced Functional Materials</i> , <b>2014</b> , 24, 2875-2882	15.6	36
87	Assessing capability of semiconductors to split water using ionization potentials and electron affinities only. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 3706-14	3.6	194
86	Non-equilibrium deposition of phase pure Cu <sub>2</sub> O thin films at reduced growth temperature. <i>APL Materials</i> , <b>2014</b> , 2, 022105	5.7	51
85	Defect Tolerant Semiconductors for Solar Energy Conversion. <i>Journal of Physical Chemistry Letters</i> , <b>2014</b> , 5, 1117-25	6.4	238
84	Experimental Characterization of a Theoretically Designed Candidate p-Type Transparent Conducting Oxide: Li-Doped Cr <sub>2</sub> MnO <sub>4</sub> . <i>Chemistry of Materials</i> , <b>2014</b> , 26, 4598-4604	9.6	13
83	Multivalency of Group 15 Dopants in SnO <sub>2</sub> . <i>Chemistry of Materials</i> , <b>2014</b> , 26, 4876-4881	9.6	11
82	Control of Doping in Cu <sub>2</sub> SnS <sub>3</sub> through Defects and Alloying. <i>Chemistry of Materials</i> , <b>2014</b> , 26, 4951-4959	9.6	119
81	Experimental Synthesis and Properties of Metastable CuNbN <sub>2</sub> and Theoretical Extension to Other Ternary Copper Nitrides. <i>Chemistry of Materials</i> , <b>2014</b> , 26, 4970-4977	9.6	44
80	Modeling amorphous thin films: Kinetically limited minimization. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	12
79	Composition Dependence of the Band Gap and Doping in Cu <sub>2</sub> O-Based Alloys as Predicted by an Extension of the Dilute-Defect Model. <i>Physical Review Applied</i> , <b>2014</b> , 2,	4.3	17
78	Polymorphism, band-structure, band-lineup, and alloy energetics of the group II oxides and sulfides MgO, ZnO, CdO, MgS, ZnS, CdS <b>2014</b> ,		3
77	Evaluation of photovoltaic materials within the Cu-Sn-S family. <i>Applied Physics Letters</i> , <b>2013</b> , 103, 253902	3.4	106
76	Convergence of density and hybrid functional defect calculations for compound semiconductors. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	77
75	Band-structure calculations for the 3d transition metal oxides in GW. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	131
74	Li-Doped Cr <sub>2</sub> MnO <sub>4</sub> : A New p-Type Transparent Conducting Oxide by Computational Materials Design. <i>Advanced Functional Materials</i> , <b>2013</b> , 23, 5267-5276	15.6	50
73	Theoretical prediction and experimental realization of new stable inorganic materials using the inverse design approach. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 10048-54	16.4	95
72	Polymorphic energy ordering of MgO, ZnO, GaN, and MnO within the random phase approximation. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	45

71	Non-equilibrium origin of high electrical conductivity in gallium zinc oxide thin films. <i>Applied Physics Letters</i> , <b>2013</b> , 103, 232106	3-4	47
70	Co <sub>3</sub> O <sub>4</sub> /Co <sub>2</sub> ZnO <sub>4</sub> spinels: The case for a solid solution. <i>Journal of Solid State Chemistry</i> , <b>2012</b> , 190, 143-149	3-3	13
69	Surface origin of high conductivities in undoped In <sub>2</sub> O <sub>3</sub> thin films. <i>Physical Review Letters</i> , <b>2012</b> , 108, 016802	7-4	96
68	Correcting density functional theory for accurate predictions of compound enthalpies of formation: Fitted elemental-phase reference energies. <i>Physical Review B</i> , <b>2012</b> , 85,	3-3	358
67	Band-structure, optical properties, and defect physics of the photovoltaic semiconductor SnS. <i>Applied Physics Letters</i> , <b>2012</b> , 100, 032104	3-4	317
66	Angle-resolved photoemission and quasiparticle calculation of ZnO: The need for d band shift in oxide semiconductors. <i>Physical Review B</i> , <b>2012</b> , 86,	3-3	49
65	Two-dimensional polaronic behavior in the binary oxides m-HfO <sub>2</sub> and m-ZrO <sub>2</sub> . <i>Physical Review Letters</i> , <b>2012</b> , 108, 116403	7-4	43
64	Prediction of A <sub>2</sub> BX <sub>4</sub> metal-chalcogenide compounds via first-principles thermodynamics. <i>Physical Review B</i> , <b>2012</b> , 86,	3-3	38
63	Band or Polaron: The Hole Conduction Mechanism in the p-Type Spinel Rh <sub>2</sub> ZnO <sub>4</sub> . <i>Journal of the American Ceramic Society</i> , <b>2012</b> , 95, 269-274	3-8	43
62	Semiconducting transition-metal oxides based on d <sup>5</sup> cations: Theory for MnO and Fe <sub>2</sub> O <sub>3</sub> . <i>Physical Review B</i> , <b>2012</b> , 85,	3-3	66
61	Cation off-stoichiometry leads to high p-type conductivity and enhanced transparency in Co <sub>2</sub> ZnO <sub>4</sub> and Co <sub>2</sub> NiO <sub>4</sub> thin films. <i>Physical Review B</i> , <b>2012</b> , 85,	3-3	67
60	Comment on "Intrinsic n-type behavior in transparent conducting oxides: a comparative hybrid-functional study of In <sub>2</sub> O <sub>3</sub> , SnO <sub>2</sub> , and ZnO". <i>Physical Review Letters</i> , <b>2011</b> , 106, 069601; author reply 069602	7-4	32
59	Inverse design approach to hole doping in ternary oxides: Enhancing p-type conductivity in cobalt oxide spinels. <i>Physical Review B</i> , <b>2011</b> , 84,	3-3	74
58	Predicting polaronic defect states by means of generalized Koopmans density functional calculations. <i>Physica Status Solidi (B): Basic Research</i> , <b>2011</b> , 248, 1052-1060	1-3	50
57	Doping Rules and Doping Prototypes in A <sub>2</sub> BO <sub>4</sub> Spinel Oxides. <i>Advanced Functional Materials</i> , <b>2011</b> , 21, 4493-4501	15-6	151
56	Iron Chalcogenide Photovoltaic Absorbers. <i>Advanced Energy Materials</i> , <b>2011</b> , 1, 748-753	21-8	128
55	Using design principles to systematically plan the synthesis of hole-conducting transparent oxides: Cu <sub>3</sub> VO <sub>4</sub> and Ag <sub>3</sub> VO <sub>4</sub> as a case study. <i>Physical Review B</i> , <b>2011</b> , 84,	3-3	34
54	Asymmetric cation nonstoichiometry in spinels: Site occupancy in Co <sub>2</sub> ZnO <sub>4</sub> and Rh <sub>2</sub> ZnO <sub>4</sub> . <i>Physical Review B</i> , <b>2011</b> , 84,	3-3	24

53	Predicting Polaronic Defect States by Means of Generalized Koopmans Density Functional Calculations <b>2011</b> , 183-199		1
52	The electronic consequences of multivalent elements in inorganic solar absorbers: Multivalency of Sn in Cu <sub>2</sub> ZnSnS <sub>4</sub> . <i>Applied Physics Letters</i> , <b>2010</b> , 96, 201902	3-4	92
51	Many-body GW calculation of the oxygen vacancy in ZnO. <i>Physical Review B</i> , <b>2010</b> , 81,	3-3	138
50	Intrinsic defects in ZnO calculated by screened exchange and hybrid density functionals. <i>Physical Review B</i> , <b>2010</b> , 81,	3-3	232
49	Dual nature of acceptors in GaN and ZnO: The curious case of the shallow MgGa deep state. <i>Applied Physics Letters</i> , <b>2010</b> , 96, 142114	3-4	88
48	Long-Range Spin Currents with Chiral Crystals. <i>Physics Magazine</i> , <b>2010</b> , 3,	1-1	180
47	Generalized Koopmans density functional calculations reveal the deep acceptor state of NO in ZnO. <i>Physical Review B</i> , <b>2010</b> , 81,	3-3	125
46	Nonstoichiometry and hole doping in NiO <b>2010</b> ,		19
45	The electronic structure of chalcopyrites Bands, point defects and grain boundaries. <i>Progress in Photovoltaics: Research and Applications</i> , <b>2010</b> , 18, 390-410	6.8	201
44	Energetics of quaternary III-V alloys described by incorporation and clustering of impurities. <i>Physical Review B</i> , <b>2009</b> , 80,	3-3	20
43	Electronic structure, donor and acceptor transitions, and magnetism of 3d impurities in In <sub>2</sub> O <sub>3</sub> and ZnO. <i>Physical Review B</i> , <b>2009</b> , 79,	3-3	93
42	Polaronic hole localization and multiple hole binding of acceptors in oxide wide-gap semiconductors. <i>Physical Review B</i> , <b>2009</b> , 80,	3-3	309
41	Electronic correlation in anion p orbitals impedes ferromagnetism due to cation vacancies in Zn chalcogenides. <i>Physical Review Letters</i> , <b>2009</b> , 103, 016404	7.4	100
40	Accurate prediction of defect properties in density functional supercell calculations. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2009</b> , 17, 084002	2	263
39	Charge self-regulation upon changing the oxidation state of transition metals in insulators. <i>Nature</i> , <b>2008</b> , 453, 763-6	50.4	199
38	Generalized valence-force-field model of (Ga,In)(N,P) ternary alloys. <i>Physical Review B</i> , <b>2008</b> , 78,	3-3	17
37	Intrinsic DX centers in ternary chalcopyrite semiconductors. <i>Physical Review Letters</i> , <b>2008</b> , 100, 016401	7.4	120
36	Relative stability, electronic structure, and magnetism of MnN and (Ga,Mn)N alloys. <i>Physical Review B</i> , <b>2008</b> , 78,	3-3	34



35	Control of ferromagnetism via electron doping in In <sub>2</sub> O <sub>3</sub> :Cr. <i>Physical Review Letters</i> , <b>2008</b> , 101, 027203	7.4	61
34	Magnetic interactions of Cr <sup>3+</sup> and Co <sup>2+</sup> impurity pairs in ZnO within a band-gap corrected density functional approach. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	128
33	Atomic control of conductivity versus ferromagnetism in wide-gap oxides via selective doping: V, Nb, Ta in anatase TiO <sub>2</sub> . <i>Physical Review Letters</i> , <b>2008</b> , 100, 036601	7.4	141
32	Assessment of correction methods for the band-gap problem and for finite-size effects in supercell defect calculations: Case studies for ZnO and GaAs. <i>Physical Review B</i> , <b>2008</b> , 78,	3.3	896
31	Limitation of the open-circuit voltage due to metastable intrinsic defects in Cu(In,Ga)Se <sub>2</sub> and strategies to avoid these defects. <i>Conference Record of the IEEE Photovoltaic Specialists Conference</i> , <b>2008</b> ,		3
30	Semiconductor thermochemistry in density functional calculations. <i>Physical Review B</i> , <b>2008</b> , 78,	3.3	98
29	Quantum-dot intermediate-band solar cells with inverted band alignment. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2008</b> , 41, 15-17	3	6
28	Origins of the doping asymmetry in oxides: Hole doping in NiO versus electron doping in ZnO. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	182
27	Origins of the p-type nature and cation deficiency in Cu <sub>2</sub> O and related materials. <i>Physical Review B</i> , <b>2007</b> , 76,	3.3	402
26	Dopability, intrinsic conductivity, and nonstoichiometry of transparent conducting oxides. <i>Physical Review Letters</i> , <b>2007</b> , 98, 045501	7.4	543
25	Nonstoichiometry as a source of magnetism in otherwise nonmagnetic oxides: Magnetically interacting cation vacancies and their percolation. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	99
24	Impurity clustering and ferromagnetic interactions that are not carrier induced in dilute magnetic semiconductors: the case of Cu <sub>2</sub> O:Co. <i>Physical Review Letters</i> , <b>2007</b> , 99, 167203	7.4	40
23	Magnetism without magnetic ions: percolation, exchange, and formation energies of magnetism-promoting intrinsic defects in CaO. <i>Physical Review Letters</i> , <b>2006</b> , 96, 107203	7.4	285
22	Light- and bias-induced metastabilities in Cu(In,Ga)Se <sub>2</sub> based solar cells caused by the (VSe-VCu) vacancy complex. <i>Journal of Applied Physics</i> , <b>2006</b> , 100, 113725	2.5	252
21	n-type doping of CuInSe <sub>2</sub> and CuGaSe <sub>2</sub> . <i>Physical Review B</i> , <b>2005</b> , 72,	3.3	384
20	Anion vacancies as a source of persistent photoconductivity in II-VI and chalcopyrite semiconductors. <i>Physical Review B</i> , <b>2005</b> , 72,	3.3	495
19	Halogen n-type doping of chalcopyrite semiconductors. <i>Applied Physics Letters</i> , <b>2005</b> , 86, 042109	3.4	29
18	Why can CuInSe <sub>2</sub> be readily equilibrium-doped n-type but the wider-gap CuGaSe <sub>2</sub> cannot?. <i>Applied Physics Letters</i> , <b>2004</b> , 85, 5860-5862	3.4	67

17	Density functional theory calculations establish the experimental evidence of the DX center atomic structure in CdTe. <i>Physical Review Letters</i> , <b>2004</b> , 92, 225504	7.4	18
16	Metal-dimer atomic reconstruction leading to deep donor states of the anion vacancy in II-VI and chalcopyrite semiconductors. <i>Physical Review Letters</i> , <b>2004</b> , 93, 156404	7.4	53
15	DX-centers in CdTe and ZnTe Observed by Locally Sensitive Probe Atoms. <i>Materials Research Society Symposia Proceedings</i> , <b>2003</b> , 763, 131		8
14	Defect interactions of group-I elements in cubic II-VI compounds. <i>Physical Review B</i> , <b>2003</b> , 68,	3.3	12
13	Optical properties of the isoelectronic trap Hg in ZnO. <i>Applied Physics Letters</i> , <b>2003</b> , 82, 3448-3450	3.4	11
12	Photoluminescence study of II-VI semiconductors by using radioactive <sup>71</sup> As dopants. <i>Physica B: Condensed Matter</i> , <b>2001</b> , 302-303, 114-122	2.8	14
11	Vacancies in CdTe: experiment and theory. <i>Physica B: Condensed Matter</i> , <b>2001</b> , 308-310, 958-962	2.8	31
10	Defect identification by means of electric field gradient calculation. <i>Physica B: Condensed Matter</i> , <b>2001</b> , 308-310, 980-984	2.8	4
9	Identification of Defects in Semiconductors via their Electric Field Gradients. <i>Hyperfine Interactions</i> , <b>2001</b> , 136/137, 453-465	0.8	0
8	Calculated Electric Field Gradients and Electronic Properties of Acceptors in CdTe. <i>Hyperfine Interactions</i> , <b>2001</b> , 136/137, 619-625	0.8	
7	Defect complexes formed with Ag atoms in CdTe, ZnTe, and ZnSe. <i>Journal of Crystal Growth</i> , <b>2000</b> , 214-215, 967-973	1.6	14
6	Group V acceptors in CdTe: Ab initio calculation of lattice relaxation and the electric-field gradient. <i>Physical Review B</i> , <b>2000</b> , 62, R2259-R2262	3.3	45
5	Defect complexes induced by diffusion of group I acceptors into CdTe. <i>Physica B: Condensed Matter</i> , <b>1999</b> , 273-274, 843-847	2.8	6
4	The Incorporation and Complex Formation of Ag Acceptors in CdTe. <i>Materials Research Society Symposia Proceedings</i> , <b>1998</b> , 510, 337		2
3	n-type doping principles for doping CuInSe <sub>2</sub> and CuGaSe <sub>2</sub> with Cl, Br, I, Mg, Zn, and Cd		2
2	Redox Defect Thermochemistry of FeAl <sub>2</sub> O <sub>4</sub> Hercynite in Water Splitting from First-Principles Methods. <i>Chemistry of Materials</i> ,	9.6	2
1	Exploring the phase space of Zn <sub>2</sub> SbN <sub>3</sub> , a novel semiconducting nitride. <i>Journal of Materials Chemistry C</i> ,	7.1	1