Stephan Lany

List of Publications by Citations

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	Assessment of correction methods for the band-gap problem and for finite-size effects in supercell defect calculations: Case studies for ZnO and GaAs. *Physical Review B*, **2008**, 78,	3.3	896
159	Dopability, intrinsic conductivity, and nonstoichiometry of transparent conducting oxides. *Physical Review Letters*, **2007**, 98, 045501	7.4	543
158	Anion vacancies as a source of persistent photoconductivity in II-VI and chalcopyrite semiconductors. *Physical Review B*, **2005**, 72,	3.3	495
157	Origins of the p-type nature and cation deficiency in Cu2O and related materials. *Physical Review B*, **2007**, 76,	3.3	402
156	n-type doping of CuInSe2 and CuGaSe2. *Physical Review B*, **2005**, 72,	3.3	384
155	Correcting density functional theory for accurate predictions of compound enthalpies of formation: Fitted elemental-phase reference energies. *Physical Review B*, **2012**, 85,	3.3	358
154	Band-structure, optical properties, and defect physics of the photovoltaic semiconductor SnS. *Applied Physics Letters*, **2012**, 100, 032104	3.4	317
153	Polaronic hole localization and multiple hole binding of acceptors in oxide wide-gap semiconductors. *Physical Review B*, **2009**, 80,	3.3	309
152	Magnetism without magnetic ions: percolation, exchange, and formation energies of magnetism-promoting intrinsic defects in CaO. *Physical Review Letters*, **2006**, 96, 107203	7.4	285
151	Accurate prediction of defect properties in density functional supercell calculations. *Modelling and Simulation in Materials Science and Engineering*, **2009**, 17, 084002	2	263
150	Light- and bias-induced metastabilities in Cu(In,Ga)Se2 based solar cells caused by the (VSe-VCu) vacancy complex. *Journal of Applied Physics*, **2006**, 100, 113725	2.5	252
149	Defect Tolerant Semiconductors for Solar Energy Conversion. *Journal of Physical Chemistry Letters*, **2014**, 5, 1117-25	6.4	238
148	Intrinsic defects in ZnO calculated by screened exchange and hybrid density functionals. *Physical Review B*, **2010**, 81,	3.3	232
147	The electronic structure of chalcopyrites-Bands, point defects and grain boundaries. *Progress in Photovoltaics: Research and Applications*, **2010**, 18, 390-410	6.8	201
146	Charge self-regulation upon changing the oxidation state of transition metals in insulators. *Nature*, **2008**, 453, 763-6	50.4	199
145	Assessing capability of semiconductors to split water using ionization potentials and electron affinities only. *Physical Chemistry Chemical Physics*, **2014**, 16, 3706-14	3.6	194
144	Origins of the doping asymmetry in oxides: Hole doping in NiO versus electron doping in ZnO. *Physical Review B*, **2007**, 75,	3.3	182

143	Long-Range Spin Currents with Chiral Crystals. *Physics Magazine*, **2010**, 3,	1.1	180
142	Predicting synthesizability. *Journal Physics D: Applied Physics*, **2019**, 52,	3	161
141	Doping Rules and Doping Prototypes in A2BO4 Spinel Oxides. *Advanced Functional Materials*, **2011**, 21, 4493-4501	15.6	151
140	A map of the inorganic ternary metal nitrides. *Nature Materials*, **2019**, 18, 732-739	27	148
139	Atomic control of conductivity versus ferromagnetism in wide-gap oxides via selective doping: V, Nb, Ta in anatase TiO2. *Physical Review Letters*, **2008**, 100, 036601	7.4	141
138	Many-body GW calculation of the oxygen vacancy in ZnO. *Physical Review B*, **2010**, 81,	3.3	138
137	Band-structure calculations for the 3d transition metal oxides in GW. *Physical Review B*, **2013**, 87,	3.3	131
136	Electronic structures of Cu2O,Cu4O3, and CuO: A joint experimental and theoretical study. *Physical Review B*, **2016**, 94,	3.3	130
135	Iron Chalcogenide Photovoltaic Absorbers. *Advanced Energy Materials*, **2011**, 1, 748-753	21.8	128
134	Magnetic interactions of Cr□Cr and Co□Co impurity pairs in ZnO within a band-gap corrected density functional approach. *Physical Review B*, **2008**, 77,	3.3	128
133	Generalized Koopmans density functional calculations reveal the deep acceptor state of NO in ZnO. *Physical Review B*, **2010**, 81,	3.3	125
132	Intrinsic DX centers in ternary chalcopyrite semiconductors. *Physical Review Letters*, **2008**, 100, 016401	7.4	120
131	Control of Doping in Cu2SnS3 through Defects and Alloying. *Chemistry of Materials*, **2014**, 26, 4951-4959	9.6	119
130	Semiconducting transition metal oxides. *Journal of Physics Condensed Matter*, **2015**, 27, 283203	1.8	111
129	Evaluation of photovoltaic materials within the Cu-Sn-S family. *Applied Physics Letters*, **2013**, 103, 253902	3.4	106
128	Electronic correlation in anion p orbitals impedes ferromagnetism due to cation vacancies in Zn chalcogenides. *Physical Review Letters*, **2009**, 103, 016404	7.4	100
127	Nonstoichiometry as a source of magnetism in otherwise nonmagnetic oxides: Magnetically interacting cation vacancies and their percolation. *Physical Review B*, **2007**, 75,	3.3	99
126	Semiconductor thermochemistry in density functional calculations. *Physical Review B*, **2008**, 78,	3.3	98

125	Self-regulated growth and tunable properties of CuSbS2 solar absorbers. *Solar Energy Materials and Solar Cells*, **2015**, 132, 499-506	6.4	97
124	Surface origin of high conductivities in undoped In2O3 thin films. *Physical Review Letters*, **2012**, 108, 016802	7.4	96
123	Theoretical prediction and experimental realization of new stable inorganic materials using the inverse design approach. *Journal of the American Chemical Society*, **2013**, 135, 10048-54	16.4	95
122	Electronic structure, donor and acceptor transitions, and magnetism of 3d impurities in In2O3 and ZnO. *Physical Review B*, **2009**, 79,	3.3	93
121	The electronic consequences of multivalent elements in inorganic solar absorbers: Multivalency of Sn in Cu2ZnSnS4. *Applied Physics Letters*, **2010**, 96, 201902	3.4	92
120	Revisiting the Valence and Conduction Band Size Dependence of PbS Quantum Dot Thin Films. *ACS Nano*, **2016**, 10, 3302-11	16.7	89
119	Dual nature of acceptors in GaN and ZnO: The curious case of the shallow MgGa deep state. *Applied Physics Letters*, **2010**, 96, 142114	3.4	88
118	Perovskite-Inspired Photovoltaic Materials: Toward Best Practices in Materials Characterization and Calculations. *Chemistry of Materials*, **2017**, 29, 1964-1988	9.6	87
117	Control of the Electrical Properties in Spinel Oxides by Manipulating the Cation Disorder. *Advanced Functional Materials*, **2014**, 24, 610-618	15.6	86
116	A computational framework for automation of point defect calculations. *Computational Materials Science*, **2017**, 130, 1-9	3.2	83
115	Physical descriptor for the Gibbs energy of inorganic crystalline solids and temperature-dependent materials chemistry. *Nature Communications*, **2018**, 9, 4168	17.4	80
114	Thermodynamic Routes to Novel Metastable Nitrogen-Rich Nitrides. *Chemistry of Materials*, **2017**, 29, 6936-6946	9.6	78
113	Convergence of density and hybrid functional defect calculations for compound semiconductors. *Physical Review B*, **2013**, 88,	3.3	77
112	Inverse design approach to hole doping in ternary oxides: Enhancing p-type conductivity in cobalt oxide spinels. *Physical Review B*, **2011**, 84,	3.3	74
111	Roadmap on optical energy conversion. *Journal of Optics (United Kingdom)*, **2016**, 18, 073004	1.7	69
110	CuSbSe2photovoltaic devices with 3% efficiency. *Applied Physics Express*, **2015**, 8, 082301	2.4	67
109	Cation off-stoichiometry leads to high p-type conductivity and enhanced transparency in Co2ZnO4 and Co2NiO4 thin films. *Physical Review B*, **2012**, 85,	3.3	67
108	Why can CuInSe2 be readily equilibrium-doped n-type but the wider-gap CuGaSe2 cannot?. *Applied Physics Letters*, **2004**, 85, 5860-5862	3.4	67

107	Semiconducting transition-metal oxides based on d5 cations: Theory for MnO and Fe2O3. *Physical Review B*, **2012**, 85,	3.3	66
106	Defect phase diagram for doping of Ga2O3. *APL Materials*, **2018**, 6, 046103	5.7	65
105	Effects of Disorder on Carrier Transport in Cu2SnS3. *Physical Review Applied*, **2015**, 4,	4.3	63
104	Accelerated development of CuSbS2 thin film photovoltaic device prototypes. *Progress in Photovoltaics: Research and Applications*, **2016**, 24, 929-939	6.8	61
103	Control of ferromagnetism via electron doping in In2O3:Cr. *Physical Review Letters*, **2008**, 101, 027203	7.4	61
102	Entropy-Driven Clustering in Tetrahedrally Bonded Multinary Materials. *Physical Review Applied*, **2015**, 3,	4.3	57
101	Monte Carlo simulations of disorder in ZnSnN2 and the effects on the electronic structure. *Physical Review Materials*, **2017**, 1,	3.2	57
100	A review of defects and disorder in multinary tetrahedrally bonded semiconductors. *Semiconductor Science and Technology*, **2016**, 31, 123004	1.8	56
99	Metal-dimer atomic reconstruction leading to deep donor states of the anion vacancy in II-VI and chalcopyrite semiconductors. *Physical Review Letters*, **2004**, 93, 156404	7.4	53
98	Non-equilibrium deposition of phase pure Cu2O thin films at reduced growth temperature. *APL Materials*, **2014**, 2, 022105	5.7	51
97	Li-Doped Cr2MnO4: A New p-Type Transparent Conducting Oxide by Computational Materials Design. *Advanced Functional Materials*, **2013**, 23, 5267-5276	15.6	50
96	Predicting polaronic defect states by means of generalized Koopmans density functional calculations. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 1052-1060	1.3	50
95	Angle-resolved photoemission and quasiparticle calculation of ZnO: The need for d band shift in oxide semiconductors. *Physical Review B*, **2012**, 86,	3.3	49
94	Effect of extended strain fields on point defect phonon scattering in thermoelectric materials. *Physical Chemistry Chemical Physics*, **2015**, 17, 19410-23	3.6	48
93	Non-equilibrium origin of high electrical conductivity in gallium zinc oxide thin films. *Applied Physics Letters*, **2013**, 103, 232106	3.4	47
92	Polymorphic energy ordering of MgO, ZnO, GaN, and MnO within the random phase approximation. *Physical Review B*, **2013**, 87,	3.3	45
91	Group V acceptors in CdTe: Ab initio calculation of lattice relaxation and the electric-field gradient. *Physical Review B*, **2000**, 62, R2259-R2262	3.3	45
90	Experimental Synthesis and Properties of Metastable CuNbN2 and Theoretical Extension to Other Ternary Copper Nitrides. *Chemistry of Materials*, **2014**, 26, 4970-4977	9.6	44

89	Two-dimensional polaronic behavior in the binary oxides m-HfO2 and m-ZrO2. *Physical Review Letters*, **2012**, 108, 116403	7.4	43
88	Band or Polaron: The Hole Conduction Mechanism in the p-Type Spinel Rh2ZnO4. *Journal of the American Ceramic Society*, **2012**, 95, 269-274	3.8	43
87	Selection Metric for Photovoltaic Materials Screening Based on Detailed-Balance Analysis. *Physical Review Applied*, **2017**, 8,	4.3	41
86	Semiconducting properties of spinel tin nitride and other IV3N4 polymorphs. *Journal of Materials Chemistry C*, **2015**, 3, 1389-1396	7.1	40
85	Impurity clustering and ferromagnetic interactions that are not carrier induced in dilute magnetic semiconductors: the case of Cu2O:Co. *Physical Review Letters*, **2007**, 99, 167203	7.4	40
84	Prediction of A2BX4 metal-chalcogenide compounds via first-principles thermodynamics. *Physical Review B*, **2012**, 86,	3.3	38
83	Novel phase diagram behavior and materials design in heterostructural semiconductor alloys. *Science Advances*, **2017**, 3, e1700270	14.3	37
82	Enhanced Electron Mobility Due to Dopant-Defect Pairing in Conductive ZnMgO. *Advanced Functional Materials*, **2014**, 24, 2875-2882	15.6	36
81	Trade-Offs in Thin Film Solar Cells with Layered Chalcostibite Photovoltaic Absorbers. *Advanced Energy Materials*, **2017**, 7, 1601935	21.8	35
80	Redox-Mediated Stabilization in Zinc Molybdenum Nitrides. *Journal of the American Chemical Society*, **2018**, 140, 4293-4301	16.4	34
79	Using design principles to systematically plan the synthesis of hole-conducting transparent oxides: Cu3VO4 and Ag3VO4 as a case study. *Physical Review B*, **2011**, 84,	3.3	34
78	Relative stability, electronic structure, and magnetism of MnN and (Ga,Mn)N alloys. *Physical Review B*, **2008**, 78,	3.3	34
77	The role of decomposition reactions in assessing first-principles predictions of solid stability. *Npj Computational Materials*, **2019**, 5,	10.9	32
76	Computationally Driven Two-Dimensional Materials Design: What Is Next?. *ACS Nano*, **2017**, 11, 7560-7564	16.7	32
75	Comment on "Intrinsic n-type behavior in transparent conducting oxides: a comparative hybrid-functional study of In2O3, SnO2, and ZnO". *Physical Review Letters*, **2011**, 106, 069601; author reply 069602	7.4	32
74	Ternary nitride semiconductors in the rocksalt crystal structure. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 14829-14834	11.5	31
73	Vacancies in CdTe: experiment and theory. *Physica B: Condensed Matter*, **2001**, 308-310, 958-962	2.8	31
72	Design of Semiconducting Tetrahedral Mn1−ZnxO Alloys and Their Application to Solar Water Splitting. *Physical Review X*, **2015**, 5,	9.1	30

71	Halogen n-type doping of chalcopyrite semiconductors. *Applied Physics Letters*, **2005**, 86, 042109	3.4	29
70	Exciton photoluminescence and benign defect complex formation in zinc tin nitride. *Materials Horizons*, **2018**, 5, 823-830	14.4	29
69	Interplay between Composition, Electronic Structure, Disorder, and Doping due to Dual Sublattice Mixing in Nonequilibrium Synthesis of ZnSnN :O. *Advanced Materials*, **2019**, 31, e1807406	24	27
68	Structural and electronic modification of photovoltaic SnS by alloying. *Journal of Applied Physics*, **2014**, 115, 113507	2.5	27
67	Negative-pressure polymorphs made by heterostructural alloying. *Science Advances*, **2018**, 4, eaaq1442	14.3	25
66	Utilizing Site Disorder in the Development of New Energy-Relevant Semiconductors. *ACS Energy Letters*, **2020**, 5, 2027-2041	20.1	24
65	Asymmetric cation nonstoichiometry in spinels: Site occupancy in Co2ZnO4 and Rh2ZnO4. *Physical Review B*, **2011**, 84,	3.3	24
64	Characterization of defects in copper antimony disulfide. *Journal of Materials Chemistry A*, **2017**, 5, 21986-21993	9.9	23
63	Synthesis of a mixed-valent tin nitride and considerations of its possible crystal structures. *Journal of Chemical Physics*, **2016**, 144, 144201	3.9	23
62	Pathway to oxide photovoltaics via band-structure engineering of SnO. *APL Materials*, **2016**, 4, 106103	5.7	23
61	Non-equilibrium alloying controls optoelectronic properties in Cu2O thin films for photovoltaic absorber applications. *Applied Physics Letters*, **2015**, 106, 123903	3.4	21
60	Understanding and Control of Bipolar Self-Doping in Copper Nitride. *Journal of Applied Physics*, **2016**, 119,	2.5	21
59	Energetics of quaternary III-V alloys described by incorporation and clustering of impurities. *Physical Review B*, **2009**, 80,	3.3	20
58	Design of Metastable Tin Titanium Nitride Semiconductor Alloys. *Chemistry of Materials*, **2017**, 29, 6511-6517	9.6	19
57	Nonstoichiometry and hole doping in NiO **2010**,		19
56	Combinatorial Synthesis of Magnesium Tin Nitride Semiconductors. *Journal of the American Chemical Society*, **2020**, 142, 8421-8430	16.4	19
55	Density functional theory calculations establish the experimental evidence of the DX center atomic structure in CdTe. *Physical Review Letters*, **2004**, 92, 225504	7.4	18
54	Composition Dependence of the Band Gap and Doping in Cu2O-Based Alloys as Predicted by an Extension of the Dilute-Defect Model. *Physical Review Applied*, **2014**, 2,	4.3	17

53	Generalized valence-force-field model of (Ga,In)(N,P) ternary alloys. *Physical Review B*, **2008**, 78,	3.3	17
52	Semiconducting cubic titanium nitride in the Th3P4 structure. *Physical Review Materials*, **2018**, 2,	3.2	17
51	Electron Doping of Proposed Kagome Quantum Spin Liquid Produces Localized States in the Band Gap. *Physical Review Letters*, **2018**, 121, 186402	7.4	17
50	Thin Film Synthesis of Semiconductors in the Mg□Sb□N Materials System. *Chemistry of Materials*, **2019**, 31, 8717-8724	9.6	16
49	Non-equilibrium synthesis, structure, and opto-electronic properties of Cu2□x Zn x O alloys. *Journal of Materials Science*, **2015**, 50, 1350-1357	4.3	16
48	Band Edge Positions and Their Impact on the Simulated Device Performance of ZnSnN2-Based Solar Cells. *IEEE Journal of Photovoltaics*, **2018**, 8, 110-117	3.7	16
47	Using heterostructural alloying to tune the structure and properties of the thermoelectric Sn1□CaxSe. *Journal of Materials Chemistry A*, **2017**, 5, 16873-16882	13	16
46	Extended antisite defects in tetrahedrally bonded semiconductors. *Physical Review B*, **2015**, 92,	3.3	16
45	Spin-orbit coupling effects on predicting defect properties with hybrid functionals: A case study in CdTe. *Physical Review B*, **2018**, 98,	3.3	15
44	Synthesis and Characterization of (Sn,Zn)O Alloys. *Chemistry of Materials*, **2016**, 28, 7765-7772	9.6	15
43	Photoluminescence study of II□VI semiconductors by using radioactive 71As dopants. *Physica B: Condensed Matter*, **2001**, 302-303, 114-122	2.8	14
42	Defect complexes formed with Ag atoms in CdTe, ZnTe, and ZnSe. *Journal of Crystal Growth*, **2000**, 214-215, 967-973	1.6	14
41	Optically induced metastability in Cu(In,Ga)Se. *Scientific Reports*, **2017**, 7, 13788	4.9	13
40	Zn2SbN3: growth and characterization of a metastable photoactive semiconductor. *Materials Horizons*, **2019**, 6, 1669-1674	14.4	13
39	Communication: The electronic entropy of charged defect formation and its impact on thermochemical redox cycles. *Journal of Chemical Physics*, **2018**, 148, 071101	3.9	13
38	Experimental Characterization of a Theoretically Designed Candidate p-Type Transparent Conducting Oxide: Li-Doped Cr2MnO4. *Chemistry of Materials*, **2014**, 26, 4598-4604	9.6	13
37	Co3O4□Co2ZnO4 spinels: The case for a solid solution. *Journal of Solid State Chemistry*, **2012**, 190, 143-149	3.3	13
36	Solubility limits in quaternary SnTe-based alloys. *RSC Advances*, **2017**, 7, 24747-24753	3.7	12

35	Electron scattering mechanisms in polycrystalline sputtered zinc tin oxynitride thin films. *Journal of Applied Physics*, **2019**, 126, 035701	2.5	12
34	Modeling amorphous thin films: Kinetically limited minimization. *Physical Review B*, **2014**, 90,	3.3	12
33	Defect interactions of group-I elements in cubic II-VI compounds. *Physical Review B*, **2003**, 68,	3.3	12
32	Combinatorial investigation of structural and optical properties of cation-disordered ZnGeN2. *Journal of Materials Chemistry C*, **2020**, 8, 8736-8746	7.1	11
31	Multivalency of Group 15 Dopants in SnO2. *Chemistry of Materials*, **2014**, 26, 4876-4881	9.6	11
30	Optical properties of the isoelectronic trap Hg in ZnO. *Applied Physics Letters*, **2003**, 82, 3448-3450	3.4	11
29	Wild band edges: The role of bandgap grading and band-edge fluctuations in high-efficiency chalcogenide devices **2016**,		10
28	Probing configurational disorder in ZnGeN2 using cluster-based Monte Carlo. *Physical Review Materials*, **2021**, 5,	3.2	10
27	Zinc-Stabilized Manganese Telluride with Wurtzite Crystal Structure. *Journal of Physical Chemistry C* , **2018**, 122, 18769-18775	3.8	9
26	The effect of sub-oxide phases on the transparency of tin-doped gallium oxide. *Applied Physics Letters*, **2016**, 109, 141909	3.4	8
25	DX-centers in CdTe and ZnTe Observed by Locally Sensitive Probe Atoms. *Materials Research Society Symposia Proceedings*, **2003**, 763, 131		8
24	Perfect short-range ordered alloy with line-compound-like properties in the ZnSnN2:ZnO system. *Npj Computational Materials*, **2020**, 6,	10.9	8
23	Computational discovery of stable and metastable ternary oxynitrides. *Journal of Chemical Physics*, **2021**, 154, 234706	3.9	7
22	ZnxMn1□O Solid Solutions in the Rocksalt Structure: Optical, Charge Transport, and Photoelectrochemical Properties. *ACS Applied Energy Materials*, **2018**, 1, 260-266	6.1	6
21	Quantum-dot intermediate-band solar cells with inverted band alignment. *Physica E: Low-Dimensional Systems and Nanostructures*, **2008**, 41, 15-17	3	6
20	Defect complexes induced by diffusion of group I acceptors into CdTe. *Physica B: Condensed Matter*, **1999**, 273-274, 843-847	2.8	6
19	Metal chalcogenides for neuromorphic computing: emerging materials and mechanisms. *Nanotechnology*, **2021**, 32,	3.4	6
18	Conduction band position tuning and Ga-doping in (Cd,Zn)S alloy thin films. *Materials Chemistry Frontiers*, **2017**, 1, 1342-1348	7.8	5

17	High-Throughput Experimental Study of Wurtzite Mn Zn O Alloys for Water Splitting Applications. *ACS Omega*, **2019**, 4, 7436-7447	3.9	4
16	Defect identification by means of electric field gradient calculation. *Physica B: Condensed Matter*, **2001**, 308-310, 980-984	2.8	4
15	Polymorphism, band-structure, band-lineup, and alloy energetics of the group II oxides and sulfides MgO, ZnO, CdO, MgS, ZnS, CdS **2014**,		3
14	Limitation of the open-circuit voltage due to metastable intrinsic defects in Cu(In,Ga)Se2 and strategies to avoid these defects. *Conference Record of the IEEE Photovoltaic Specialists Conference*, **2008**,		3
13	Templated Growth of Metastable Polymorphs on Amorphous Substrates with Seed Layers. *Physical Review Applied*, **2020**, 13,	4.3	3
12	n-type doping principles for doping CuInSe/sub 2/ and CuGaSe/sub 2/ with Cl, Br, I, Mg, Zn, and Cd		2
11	The Incorporation and Complex Formation of Ag Acceptors in CdTe. *Materials Research Society Symposia Proceedings*, **1998**, 510, 337		2
10	Redox Defect Thermochemistry of FeAl2O4 Hercynite in Water Splitting from First-Principles Methods. *Chemistry of Materials*,	9.6	2
9	Computational Fermi level engineering and doping-type conversion of Mg:Ga2O3 via three-step synthesis process. *Journal of Applied Physics*, **2021**, 129, 245704	2.5	2
8	Predicting Polaronic Defect States by Means of Generalized Koopmans Density Functional Calculations **2011**, 183-199		1
7	Bandgap analysis and carrier localization in cation-disordered ZnGeN2. *APL Materials*, **2022**, 10, 011112	5.7	1
6	Exploring the phase space of Zn2SbN3, a novel semiconducting nitride. *Journal of Materials Chemistry C*,	7.1	1
5	Short-Range Order Tunes Optical Properties in Long-Range Disordered ZnSnN2–ZnO Alloy. *Chemistry of Materials*, **2022**, 34, 3910-3919	9.6	1
4	Computational Materials Design: Interplay between Composition, Electronic Structure, Disorder, and Doping due to Dual Sublattice Mixing in Nonequilibrium Synthesis of ZnSnN2:O (Adv. Mater. 11/2019). *Advanced Materials*, **2019**, 31, 1970080	24	0
3	Wurtzite materials in alloys of rock salt compounds. *Journal of Materials Research*, **2020**, 35, 972-980	2.5	0
2	Identification of Defects in Semiconductors via their Electric Field Gradients. *Hyperfine Interactions*, **2001**, 136/137, 453-465	0.8	0
1	Calculated Electric Field Gradients and Electronic Properties of Acceptors in CdTe. *Hyperfine Interactions*, **2001**, 136/137, 619-625	0.8	