Stephan Lany

List of Publications by Year
in descending order

188	15,342	18341 62	18533 120
papers	citations	h-index	g-index

193	193	193	16626
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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	1,064
2	Dopability, Intrinsic Conductivity, and Nonstoichiometry of Transparent Conducting Oxides. Physical Review Letters, 2007, 98, 045501.	8.0	590
3	Anion vacancies as a source of persistent photoconductivity in II-VI and chalcopyrite semiconductors. Physical Review B, 2005, 72, .	3.3	580
4	Correcting density functional theory for accurate predictions of compound enthalpies of formation: Fitted elemental-phase reference energies. Physical Review B, 2012, 85, .	3.3	483
5	Origins of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>p</mml:mi></mml:math>-type nature and cation deficiency in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Cu</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi></mml:mrow></mml:math> and related materials. Physical Review B, 2007, 76, .	3.3	475
6	n-type doping ofCuInSe2andCuGaSe2. Physical Review B, 2005, 72, .	3.3	433
7	Band-structure, optical properties, and defect physics of the photovoltaic semiconductor SnS. Applied Physics Letters, 2012, 100, .	3.2	390
8	Polaronic hole localization and multiple hole binding of acceptors in oxide wide-gap semiconductors. Physical Review B, 2009, 80, .	3.3	358
9	Accurate prediction of defect properties in density functional supercell calculations. Modelling and Simulation in Materials Science and Engineering, 2009, 17, 084002.	1.9	339
10	Defect Tolerant Semiconductors for Solar Energy Conversion. Journal of Physical Chemistry Letters, 2014, 5, 1117-1125.	4.9	318
11	Magnetism without Magnetic Ions: Percolation, Exchange, and Formation Energies of Magnetism-Promoting Intrinsic Defects in CaO. Physical Review Letters, 2006, 96, 107203.	8.0	313
12	Light- and bias-induced metastabilities in Cu(In,Ga)Se[sub 2] based solar cells caused by the (V[sub) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	2.3	312
13	A map of the inorganic ternary metal nitrides. Nature Materials, 2019, 18, 732-739.	26.6	309
14	Charge self-regulation upon changing the oxidation state of transition metals in insulators. Nature, 2008, 453, 763-766.	36.2	249
15	The 2019 materials by design roadmap. Journal Physics D: Applied Physics, 2019, 52, 013001.	2.9	249
16	Intrinsic defects in ZnO calculated by screened exchange and hybrid density functionals. Physical Review B, 2010, 81, .	3.3	245
17	The electronic structure of chalcopyritesâ€"bands, point defects and grain boundaries. Progress in Photovoltaics: Research and Applications, 2010, 18, 390-410.	5.3	239
18	Assessing capability of semiconductors to split water using ionization potentials and electron affinities only. Physical Chemistry Chemical Physics, 2014, 16, 3706.	2.9	231

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19	Origins of the doping asymmetry in oxides: Hole doping in NiO versus electron doping in ZnO. Physical Review B, 2007, 75, .	3.3	225
20	Electronic structures of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:msub><mml:mi mathvariant="normal">u</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mo>,</mml:mo><mml:mi mathvariant="normal">C</mml:mi><mml:msub><mml:mi mathvariant="normal">u</mml:mi><mml:mn>4	3.3	219
21	The quest for dilute ferromagnetism in semiconductors: Guides and misguides by theory. Physics Magazine, 0, 3, .	0.1	201
22	Doping Rules and Doping Prototypes in A₂BO₄ Spinel Oxides. Advanced Functional Materials, 2011, 21, 4493-4501.	16.5	178
23	Semiconducting transition metal oxides. Journal of Physics Condensed Matter, 2015, 27, 283203.	1.9	176
24	Physical descriptor for the Gibbs energy of inorganic crystalline solids and temperature-dependent materials chemistry. Nature Communications, 2018, 9, 4168.	13.2	173
25	Band-structure calculations for the 3<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>d</mml:mi></mml:math>transition metal oxides in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>.	3.3	169
26	Atomic Control of Conductivity Versus Ferromagnetism in Wide-Gap Oxides Via Selective Doping: V, Nb, Ta in Anatase<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2008, 100, 036601.	8.0	162
27	A computational framework for automation of point defect calculations. Computational Materials Science, 2017, 130, 1-9.	3.1	150
28	Many-body<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>calculation of the oxygen vacancy in ZnO. Physical Review B, 2010, 81, .	3.3	147
29	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Cr</mml:mi><mml:mtext>â</mml:mtext><mml:mi>Cr</mml:mi></mml:mrow></mml:math>ar<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Co</mml:mi><mml:mtext>â</mml:mtext><mml:mi>Co</mml:mi></mml:mrow></mml:math>in pairs in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>ZnO</mml:mi></mml:mrow></mml:math>within Physical	3.8	146
30	Intrinsic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>D</mml:mi><mml:mi>X</mml:mi></mml:math>Centers in Ternary Chalcopyrite Semiconductors. Physical Review Letters, 2008, 100, 016401.	8.0	142
31	Iron Chalcogenide Photovoltaic Absorbers. Advanced Energy Materials, 2011, 1, 748-753.	22.2	141
32	Control of Doping in Cu₂SnS₃ through Defects and Alloying. Chemistry of Materials, 2014, 26, 4951-4959.	7.1	138
33	Generalized Koopmans density functional calculations reveal the deep acceptor state of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>N</mml:mtext><mml:mtext>O</mml:mtext></mml:msub></mml:mrow></mml:math>in ZnO. Physical Review B, 2010, 81, .	3.3	137
34	Thermodynamic Routes to Novel Metastable Nitrogen-Rich Nitrides. Chemistry of Materials, 2017, 29, 6936-6946.	7.1	130
35	Self-regulated growth and tunable properties of CuSbS2 solar absorbers. Solar Energy Materials and Solar Cells, 2015, 132, 499-506.	6.3	125
36	Revisiting the Valence and Conduction Band Size Dependence of PbS Quantum Dot Thin Films. ACS Nano, 2016, 10, 3302-3311.	15.3	124

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37	Evaluation of photovoltaic materials within the Cu-Sn-S family. Applied Physics Letters, 2013, 103, .	3.2	120
38	Perovskite-Inspired Photovoltaic Materials: Toward Best Practices in Materials Characterization and Calculations. Chemistry of Materials, 2017, 29, 1964-1988.	7.1	119
39	Semiconductor thermochemistry in density functional calculations. Physical Review B, 2008, 78, .	3.3	117
40	The electronic consequences of multivalent elements in inorganic solar absorbers: Multivalency of Sn in Cu2ZnSnS4. Applied Physics Letters, 2010, 96, .	3.2	117
41	Surface Origin of High Conductivities in Undoped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>In</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>Thin Films. Physical Review Letters, 2012, 108, 016802.	8.0	115
42	Control of the Electrical Properties in Spinel Oxides by Manipulating the Cation Disorder. Advanced Functional Materials, 2014, 24, 610-618.	16.5	114
43	Theoretical Prediction and Experimental Realization of New Stable Inorganic Materials Using the Inverse Design Approach. Journal of the American Chemical Society, 2013, 135, 10048-10054.	14.6	113
44	Nonstoichiometry as a source of magnetism in otherwise nonmagnetic oxides: Magnetically interacting cation vacancies and their percolation. Physical Review B, 2007, 75, .	3.3	110
45	Electronic structure, donor and acceptor transitions, and magnetism of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math>impurities in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>In</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub>	3.3	105
46	Electronic Correlation in Anion<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>p</mml:mi></mml:math>Orbitals Impedes Ferromagnetism due to Cation Vacancies in Zn Chalcogenides. Physical Review Letters, 2009, 103, 016404.	8.0	104
47	Dual nature of acceptors in GaN and ZnO: The curious case of the shallow MgGa deep state. Applied Physics Letters, 2010, 96, .	3.2	102
48	Defect phase diagram for doping of Ga2O3. APL Materials, 2018, 6, .	4.8	101
49	Convergence of density and hybrid functional defect calculations for compound semiconductors. Physical Review B, 2013, 88, .	3.3	100
50	Roadmap on optical energy conversion. Journal of Optics (United Kingdom), 2016, 18, 073004.	2.2	88
51	Monte Carlo simulations of disorder in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>ZnSn</mml:mi><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> and the effects on the electronic structure. Physical Review Materials, 2017, 1, .	2.5	83
52	Inverse design approach to hole doping in ternary oxides: Enhancing<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>p</mml:mi></mml:math>-type conductivity in cobalt oxide spinels. Physical Review B, 2011, 84, .	3.3	82
53	CuSbSe₂photovoltaic devices with 3% efficiency. Applied Physics Express, 2015, 8, 082301.	2.4	81
54	Accelerated development of CuSbS₂ thin film photovoltaic device prototypes. Progress in Photovoltaics: Research and Applications, 2016, 24, 929-939.	5.3	77

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55	ducting transition-metal oxides based on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mi>d</mml:mi><mml:mn>5</mml:mn></mml:msup></mml:math>cations: Theory for MnO and Fe<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>O<mml:math	3.3	75
56	Effects of Disorder on Carrier Transport in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:msub><mml:mrow><mml:mi>Cu</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn> Physical Review Applied, 2015, 4, .	3.8	75
57	A review of defects and disorder in multinary tetrahedrally bonded semiconductors. Semiconductor Science and Technology, 2016, 31, 123004.	2.1	75
58	Control of Ferromagnetism via Electron Doping in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>In</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:mo>â¶</mml:mo><mml:mi>Cr</mml:mi></mml:math>. Physical Review Letters, 2008, 101, 037203.	8.0	73
59	<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>-type conductivity and enhanced transparency in Co<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>ZnO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow />	3.3	73
60	Why can CuInSe2 be readily equilibrium-doped n-type but the wider-gap CuGaSe2 cannot?. Applied Physics Letters, 2004, 85, 5860-5862.	3.2	72
61	The role of decomposition reactions in assessing first-principles predictions of solid stability. Npj Computational Materials, 2019, 5, .	9.1	71
62	Tradeâ€Offs in Thin Film Solar Cells with Layered Chalcostibite Photovoltaic Absorbers. Advanced Energy Materials, 2017, 7, 1601935.	22.2	66
63	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.	8.0	65
64	Predicting polaronic defect states by means of generalized Koopmans density functional calculations. Physica Status Solidi (B): Basic Research, 2011, 248, 1052-1060.	1.6	63
65	Entropy-Driven Clustering in Tetrahedrally Bonded Multinary Materials. Physical Review Applied, 2015, 3, .	3.8	62
66	Two-Dimensional Polaronic Behavior in the Binary Oxides<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>m</mml:mi><mml:mtext mathvariant="normal">â^'</mml:mtext><mml:msub><mml:mi>HfO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>and<m xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>m</mml:mi><mml:mtext mathvariant="normal">â^'</mml:mtext><mml:msub><mml:mi>ZrO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2012, 108, 116403.	8.0	60
67	Liâ€Doped Cr₂MnO₄: A New pâ€Type Transparent Conducting Oxide by Computational Materials Design. Advanced Functional Materials, 2013, 23, 5267-5276.	16.5	60
68	Angle-resolved photoemission and quasiparticle calculation of ZnO: The need for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>d</mml:mi></mml:math>band shift in oxide semiconductors. Physical Review B, 2012, 86, .	3.3	57
69	Experimental Synthesis and Properties of Metastable CuNbN₂ and Theoretical Extension to Other Ternary Copper Nitrides. Chemistry of Materials, 2014, 26, 4970-4977.	7.1	57
70	Redox-Mediated Stabilization in Zinc Molybdenum Nitrides. Journal of the American Chemical Society, 2018, 140, 4293-4301.	14.6	57
71	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.	7.6	57
72	Effect of extended strain fields on point defect phonon scattering in thermoelectric materials. Physical Chemistry Chemical Physics, 2015, 17, 19410-19423.	2.9	56

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73	Non-equilibrium deposition of phase pure Cu2O thin films at reduced growth temperature. APL Materials, 2014, 2, .	4.8	55
74	Selection Metric for Photovoltaic Materials Screening Based on Detailed-Balance Analysis. Physical Review Applied, 2017, 8, .	3.8	55
75	Utilizing Site Disorder in the Development of New Energy-Relevant Semiconductors. ACS Energy Letters, 2020, 5, 2027-2041.	18.4	53
76	Polymorphic energy ordering of MgO, ZnO, GaN, and MnO within the random phase approximation. Physical Review B, 2013, 87, .	3.3	52
77	Enhanced Electron Mobility Due to Dopantâ€Defect Pairing in Conductive ZnMgO. Advanced Functional Materials, 2014, 24, 2875-2882.	16.5	52
78	Non-equilibrium origin of high electrical conductivity in gallium zinc oxide thin films. Applied Physics Letters, 2013, 103, .	3.2	51
79	Thin Film Synthesis of Semiconductors in the Mgâ€“Sbâ€“N Materials System. Chemistry of Materials, 2019, 31, 8717-8724.	7.1	50
80	Group V acceptors in CdTe:Ab initiocalculation of lattice relaxation and the electric-field gradient. Physical Review B, 2000, 62, R2259-R2262.	3.3	49
81	Semiconducting properties of spinel tin nitride and other IV₃N₄polymorphs. Journal of Materials Chemistry C, 2015, 3, 1389-1396.	5.6	49
82	Band or Polaron: The Hole Conduction Mechanism in the pâ€Type Spinel <scp><scp>Rh₂ZnO₄</scp></scp>. Journal of the American Ceramic Society, 2012, 95, 269-274.	3.8	48
83	Impurity Clustering and Ferromagnetic Interactions that are not Carrier Induced in Dilute Magnetic Semiconductors: The Case ofCu2Oâˆ¶Co. Physical Review Letters, 2007, 99, 167203.	8.0	47
84	Novel phase diagram behavior and materials design in heterostructural semiconductor alloys. Science Advances, 2017, 3, e1700270.	10.9	47
85	Prediction of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>A</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi>B</mml:mi><mml:m compounds via first-principles thermodynamics. Physical Review B, 2012, 86, .	3.3	46
86	Computationally Driven Two-Dimensional Materials Design: What Is Next?. ACS Nano, 2017, 11, 7560-7564.	15.3	44
87	Combinatorial Synthesis of Magnesium Tin Nitride Semiconductors. Journal of the American Chemical Society, 2020, 142, 8421-8430.	14.6	44
88	Exciton photoluminescence and benign defect complex formation in zinc tin nitride. Materials Horizons, 2018, 5, 823-830.	12.8	42
89	Relative stability, electronic structure, and magnetism of MnN and (Ga,Mn)N alloys. Physical Review B, 2008, 78, .	3.3	40
90	Using design principles to systematically plan the synthesis of hole-conducting transparent oxides: Cu<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>VO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>and Ag<mml:math xmlns:mml="http://www.w3.org/199	3.3	40

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91	Experimental Synthesis of Theoretically Predicted Multivalent Ternary Nitride Materials. Chemistry of Materials, 2022, 34, 1418-1438.	7.1	39
92	Negative-pressure polymorphs made by heterostructural alloying. Science Advances, 2018, 4, eaaq1442.	10.9	38
93	Interplay between Composition, Electronic Structure, Disorder, and Doping due to Dual Sublattice Mixing in Nonequilibrium Synthesis of ZnSnN₂:O. Advanced Materials, 2019, 31, e1807406.	24.3	38
94	Halogen n-type doping of chalcopyrite semiconductors. Applied Physics Letters, 2005, 86, 042109.	3.2	37
95	Zn₂SbN₃: growth and characterization of a metastable photoactive semiconductor. Materials Horizons, 2019, 6, 1669-1674.	12.8	36
96	Characterization of defects in copper antimony disulfide. Journal of Materials Chemistry A, 2017, 5, 21986-21993.	10.5	35
97	Vacancies in CdTe: experiment and theory. Physica B: Condensed Matter, 2001, 308-310, 958-962.	2.8	34
98	Design of Semiconducting Tetrahedral<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Mn</mml:mi></mml:mrow><mml:mrow><mml:mn>1</mml:mn><mn mathvariant="normal">O</mml:mi></mml:mrow></mml:math>Alloys and Their Application to Solar Water Splitting. Physical Review X, 2015, 5, .	9.1	34
99	Origin of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>n</mml:mi></mml:math>-type Behavior in Transparent Conducting Oxides: A Comparative Hybrid-Functional Study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>In</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline">	8.0	33
100	Synthesis of a mixed-valent tin nitride and considerations of its possible crystal structures. Journal of Chemical Physics, 2016, 144, 144201.	3.1	32
101	Understanding and control of bipolar self-doping in copper nitride. Journal of Applied Physics, 2016, 119, .	2.3	31
102	Structural and electronic modification of photovoltaic SnS by alloying. Journal of Applied Physics, 2014, 115, .	2.3	30
103	Pathway to oxide photovoltaics via band-structure engineering of SnO. APL Materials, 2016, 4, 106103.	4.8	29
104	Communication: The electronic entropy of charged defect formation and its impact on thermochemical redox cycles. Journal of Chemical Physics, 2018, 148, 071101.	3.1	29
105	Combinatorial investigation of structural and optical properties of cation-disordered ZnGeN₂. Journal of Materials Chemistry C, 2020, 8, 8736-8746.	5.6	29
106	Design of Metastable Tin Titanium Nitride Semiconductor Alloys. Chemistry of Materials, 2017, 29, 6511-6517.	7.1	28
107	Computational discovery of stable and metastable ternary oxynitrides. Journal of Chemical Physics, 2021, 154, 234706.	3.1	28
108	Band Edge Positions and Their Impact on the Simulated Device Performance of ZnSnN2-Based Solar Cells. IEEE Journal of Photovoltaics, 2018, 8, 110-117.	2.7	27

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109	Non-equilibrium alloying controls optoelectronic properties in Cu2O thin films for photovoltaic absorber applications. Applied Physics Letters, 2015, 106, 123903.	3.2	26
110	Spin-orbit coupling effects on predicting defect properties with hybrid functionals: A case study in CdTe. Physical Review B, 2018, 98, .	3.3	26
111	Probing configurational disorder in <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> using cluster-based Monte Carlo. Physical Review Materials, 2021, 5, .	2.5	26
112	Nonstoichiometry and hole doping in NiO. AIP Conference Proceedings, 2010, , .	1.0	25
113	Asymmetric cation nonstoichiometry in spinels: Site occupancy in Co<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>ZnO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>and Rh<mml:math	3.3	25
114	Semiconducting cubic titanium nitride in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Th</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">P</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>structure. Physical Review Materials, 2018, 2, .	2.5	25
115	Energetics of quaternary III-V alloys described by incorporation and clustering of impurities. Physical Review B, 2009, 80, .	3.3	24
116	Electron Doping of Proposed Kagome Quantum Spin Liquid Produces Localized States in the Band Gap. Physical Review Letters, 2018, 121, 186402.	8.0	23
117	Metal chalcogenides for neuromorphic computing: emerging materials and mechanisms. Nanotechnology, 2021, 32, 372001.	2.7	23
118	Perfect short-range ordered alloy with line-compound-like properties in the ZnSnN2:ZnO system. Npj Computational Materials, 2020, 6, .	9.1	22
119	Compositionally Complex Perovskite Oxides for Solar Thermochemical Water Splitting. Chemistry of Materials, 2023, 35, 1901-1915.	7.1	22
120	Role of disorder in the synthesis of metastable zinc zirconium nitrides. Physical Review Materials, 2022, 6, .	2.5	21
121	Using heterostructural alloying to tune the structure and properties of the thermoelectric Sn_{1â^'x}Ca_xSe. Journal of Materials Chemistry A, 2017, 5, 16873-16882.	10.5	20
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