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	Predicting Thermochemical Equilibria with Interacting Defects: <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mi>Sr</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn><mml:mo>â^’</mml:mo><mml:mi>Î´</mml:mi></mml:mrow></mml:msub></mml:math>. , 2024, 3, .		
2	Comparing the influence of cation order and composition in simulated Zn(Sn, Ge)N2 on structure, elastic moduli, and polarization for solid state lighting. Journal of Applied Physics, 2024, 135, .	2.3	0
3	Local Ordering, Distortion, and Redox Activity in (La_{0.75}Sr_{0.25})(Mn_{0.25}Fe_{0.25}Co_{0.25}Al_{0.25})O₃ Investigated by a Computational Workflow for Compositionally Complex Perovskite Oxides. Chemistry of Materials, 2024, 36, 4990-5001.	7.1	0
4	Chemical Potential Analysis as an Alternative to the vanâ€™t Hoff Method: Hypothetical Limits of Solar Thermochemical Hydrogen. Journal of the American Chemical Society, 2024, 146, 14114-14127.	14.6	0
5	Heterostructural alloy phase diagram for (<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 587 Td (xmlns:mml="http://www.v Physical Review Materials, 2024, 8, .	2.5	0
6	Tutorial: Defects in topological semimetals. Journal of Applied Physics, 2024, 136, .	2.3	0
7	Computational discovery of two-dimensional rare-earth iodides: promising ferrovalley materials for valleytronics. 2D Materials, 2023, 10, 015021.	4.5	10
8	Combinatorial Synthesis of Cation-Disordered Manganese Tin Nitride MnSnN₂ Thin Films with Magnetic and Semiconducting Properties. Chemistry of Materials, 2023, 35, 2936-2946.	7.1	7
9	Extrinsic n-type doping of Cd₃As₂ thin films. Applied Physics Letters, 2023, 122, 061901.	3.2	0
10	Investigating the Electronic Structure of Prospective Water-Splitting Oxide BaCe_{0.25}Mn_{0.75}O_{3â^’Î´} before and after Thermal Reduction. Chemistry of Materials, 2023, 35, 1935-1947.	7.1	1
11	Compositionally Complex Perovskite Oxides for Solar Thermochemical Water Splitting. Chemistry of Materials, 2023, 35, 1901-1915.	7.1	22
12	Accurate prediction of oxygen vacancy concentration with disordered A-site cations in high-entropy perovskite oxides. Npj Computational Materials, 2023, 9, .	9.1	12
13	Direct link between disorder and magnetoresistance in topological semimetals. Physical Review B, 2023, 107, .	3.3	4
14	Band energy dependence of defect formation in the topological semimetal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>Cd</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn> Physical Review B, 2023, 107, .	3.3	2
15	Defect graph neural networks for materials discovery in high-temperature clean-energy applications. Nature Computational Science, 2023, 3, 675-686.	5.6	15
16	Sampling and screening approaches for imperfect materials: Defects and incommensurate interfaces. , 2023, , .		0
17	From data-driven modeling to systems level co-design: progress in materials discovery and optimization for hydrogen storage and generation. , 2023, , .		0
18	Redox Defect Thermochemistry of FeAl₂O₄ Hercynite in Water Splitting from First-Principles Methods. Chemistry of Materials, 2022, 34, 519-528.	7.1	16

#	Article	IF	Citations
19	Bandgap analysis and carrier localization in cation-disordered ZnGeN2. APL Materials, 2022, 10, .	4.8	16
20	Experimental Synthesis of Theoretically Predicted Multivalent Ternary Nitride Materials. Chemistry of Materials, 2022, 34, 1418-1438.	7.1	39
21	Formation of 6H-Ba₃Ce_{0.75}Mn_{2.25}O₉ during Thermochemical Reduction of 12R-Ba₄CeMn₃O₁₂: Identification of a Polytype in the Ba(Ce,Mn)O₃ Family. Inorganic Chemistry, 2022, 61, 6128-6137.	4.2	7
22	Role of disorder in the synthesis of metastable zinc zirconium nitrides. Physical Review Materials, 2022, 6, .	2.5	21
23	Short-Range Order Tunes Optical Properties in Long-Range Disordered ZnSnN₂â€“ZnO Alloy. Chemistry of Materials, 2022, 34, 3910-3919.	7.1	6
24	Simulation and characterization of cation disorder in $$hbox {ZnGeP}_{2}$$. Journal of Materials Research, 2022, 37, 1986-1996.	2.6	3
25	Structural, Vibrational, and Electronic Properties of Cation-Disordered <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mrow><mml:mi>Zn</mml:mi><mml:mi>Ge</mml:mi><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math> <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mi /><mml:mn>2</mml:mn></mml:msub></mml:math> and its Inte...	3.8	4
26	Atomically thin interlayer phase from first principles enables defect-free incommensurate SnO2/CdTe interface. Applied Physics Reviews, 2022, 9, .	11.7	1
27	Exploring the phase space of Zn₂SbN₃, a novel semiconducting nitride. Journal of Materials Chemistry C, 2021, 9, 13904-13913.	5.6	7
28	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></m using cluster-based Monte Carlo. Physical Review Materials, 2021, 5, .	2.5	26
29	Computational discovery of stable and metastable ternary oxynitrides. Journal of Chemical Physics, 2021, 154, 234706.	3.1	28
30	First principles predictions of SnO2/CdTe and SnO2/CdCl2/CdTe interface structures. , 2021, , .		0
31	Computational Fermi level engineering and doping-type conversion of Mg:Ga2O3 via three-step synthesis process. Journal of Applied Physics, 2021, 129, .	2.3	15
32	Metal chalcogenides for neuromorphic computing: emerging materials and mechanisms. Nanotechnology, 2021, 32, 372001.	2.7	23
33	A New Class of High Entropy Perovskite Oxides with Increased Reducibility and Stability for Solar Thermochemical Hydrogen Production. ECS Meeting Abstracts, 2021, MA2021-02, 1354-1354.	0.0	1
34	Templated Growth of Metastable Polymorphs on Amorphous Substrates with Seed Layers. Physical Review Applied, 2020, 13, .	3.8	8
35	Perfect short-range ordered alloy with line-compound-like properties in the ZnSnN2:ZnO system. Npj Computational Materials, 2020, 6, .	9.1	22
36	Combinatorial investigation of structural and optical properties of cation-disordered ZnGeN₂. Journal of Materials Chemistry C, 2020, 8, 8736-8746.	5.6	29

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37	Wurtzite materials in alloys of rock salt compounds. Journal of Materials Research, 2020, 35, 972-980.	2.6	2
38	Utilizing Site Disorder in the Development of New Energy-Relevant Semiconductors. ACS Energy Letters, 2020, 5, 2027-2041.	18.4	53
39	Combinatorial Synthesis of Magnesium Tin Nitride Semiconductors. Journal of the American Chemical Society, 2020, 142, 8421-8430.	14.6	44
40	The 2019 materials by design roadmap. Journal Physics D: Applied Physics, 2019, 52, 013001.	2.9	249
41	Electron scattering mechanisms in polycrystalline sputtered zinc tin oxynitride thin films. Journal of Applied Physics, 2019, 126, 035701.	2.3	13
42	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
43	Thin Film Synthesis of Semiconductors in the Mgâ€“Sbâ€“N Materials System. Chemistry of Materials, 2019, 31, 8717-8724.	7.1	50
44	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
45	The role of decomposition reactions in assessing first-principles predictions of solid stability. Npj Computational Materials, 2019, 5, .	9.1	71
46	A map of the inorganic ternary metal nitrides. Nature Materials, 2019, 18, 732-739.	26.6	309
47	High-Throughput Experimental Study of Wurtzite Mn_{1â€“x}Zn_xO Alloys for Water Splitting Applications. ACS Omega, 2019, 4, 7436-7447.	3.6	6
48	Zn₂SbN₃: growth and characterization of a metastable photoactive semiconductor. Materials Horizons, 2019, 6, 1669-1674.	12.8	36
49	Redox-Mediated Stabilization in Zinc Molybdenum Nitrides. Journal of the American Chemical Society, 2018, 140, 4293-4301.	14.6	57
50	Negative-pressure polymorphs made by heterostructural alloying. Science Advances, 2018, 4, eaaq1442.	10.9	38
51	Defect phase diagram for doping of Ga2O3. APL Materials, 2018, 6, .	4.8	101
52	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
53	Zn_xMn_{1â€“x}O Solid Solutions in the Rocksalt Structure: Optical, Charge Transport, and Photoelectrochemical Properties. ACS Applied Energy Materials, 2018, 1, 260-266.	5.3	8
54	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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55	Physical descriptor for the Gibbs energy of inorganic crystalline solids and temperature-dependent materials chemistry. Nature Communications, 2018, 9, 4168.	13.2	173
56	Electron Doping of Proposed Kagome Quantum Spin Liquid Produces Localized States in the Band Gap. Physical Review Letters, 2018, 121, 186402.	8.0	23
57	Exciton photoluminescence and benign defect complex formation in zinc tin nitride. Materials Horizons, 2018, 5, 823-830.	12.8	42
58	Zinc-Stabilized Manganese Telluride with Wurtzite Crystal Structure. Journal of Physical Chemistry C, 2018, 122, 18769-18775.	3.3	15
59	Spin-orbit coupling effects on predicting defect properties with hybrid functionals: A case study in CdTe. Physical Review B, 2018, 98, .	3.3	26
60	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: 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
61	Perovskite-Inspired Photovoltaic Materials: Toward Best Practices in Materials Characterization and Calculations. Chemistry of Materials, 2017, 29, 1964-1988.	7.1	119
62	A computational framework for automation of point defect calculations. Computational Materials Science, 2017, 130, 1-9.	3.1	150
63	Tradeâ€Offs in Thin Film Solar Cells with Layered Chalcostibite Photovoltaic Absorbers. Advanced Energy Materials, 2017, 7, 1601935.	22.2	66
64	Conduction band position tuning and Ga-doping in (Cd,Zn)S alloy thin films. Materials Chemistry Frontiers, 2017, 1, 1342-1348.	5.9	6
65	Solubility limits in quaternary SnTe-based alloys. RSC Advances, 2017, 7, 24747-24753.	3.7	14
66	Novel phase diagram behavior and materials design in heterostructural semiconductor alloys. Science Advances, 2017, 3, e1700270.	10.9	47
67	Optically induced metastability in Cu(In,Ga)Se2. Scientific Reports, 2017, 7, 13788.	3.4	18
68	Selection Metric for Photovoltaic Materials Screening Based on Detailed-Balance Analysis. Physical Review Applied, 2017, 8, .	3.8	55
69	Characterization of defects in copper antimony disulfide. Journal of Materials Chemistry A, 2017, 5, 21986-21993.	10.5	35
70	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
71	Thermodynamic Routes to Novel Metastable Nitrogen-Rich Nitrides. Chemistry of Materials, 2017, 29, 6936-6946.	7.1	130
72	Computationally Driven Two-Dimensional Materials Design: What Is Next?. ACS Nano, 2017, 11, 7560-7564.	15.3	44

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73	Design of Metastable Tin Titanium Nitride Semiconductor Alloys. Chemistry of Materials, 2017, 29, 6511-6517.	7.1	28
74	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
75	Wild band edges: The role of bandgap grading and band-edge fluctuations in high-efficiency chalcogenide devices. , 2016, , .		11
76	A review of defects and disorder in multinary tetrahedrally bonded semiconductors. Semiconductor Science and Technology, 2016, 31, 123004.	2.1	75
77	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</mml:mn>	3.3	219
78	Synthesis of a mixed-valent tin nitride and considerations of its possible crystal structures. Journal of Chemical Physics, 2016, 144, 144201.	3.1	32
79	Understanding and control of bipolar self-doping in copper nitride. Journal of Applied Physics, 2016, 119, .	2.3	31
80	Pathway to oxide photovoltaics via band-structure engineering of SnO. APL Materials, 2016, 4, 106103.	4.8	29
81	Synthesis and Characterization of (Sn,Zn)O Alloys. Chemistry of Materials, 2016, 28, 7765-7772.	7.1	16
82	The effect of sub-oxide phases on the transparency of tin-doped gallium oxide. Applied Physics Letters, 2016, 109, .	3.2	9
83	Accelerated development of CuSbS₂ thin film photovoltaic device prototypes. Progress in Photovoltaics: Research and Applications, 2016, 24, 929-939.	5.3	77
84	Roadmap on optical energy conversion. Journal of Optics (United Kingdom), 2016, 18, 073004.	2.2	88
85	Revisiting the Valence and Conduction Band Size Dependence of PbS Quantum Dot Thin Films. ACS Nano, 2016, 10, 3302-3311.	15.3	124
86	Entropy-Driven Clustering in Tetrahedrally Bonded Multinary Materials. Physical Review Applied, 2015, 3, .	3.8	62
87	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
88	Extended antisite defects in tetrahedrally bonded semiconductors. Physical Review B, 2015, 92, .	3.3	17
89	CuSbSe₂photovoltaic devices with 3% efficiency. Applied Physics Express, 2015, 8, 082301.	2.4	81
90	Semiconducting properties of spinel tin nitride and other IV₃N₄polymorphs. Journal of Materials Chemistry C, 2015, 3, 1389-1396.	5.6	49

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91	Non-equilibrium synthesis, structure, and opto-electronic properties of Cu2â^'2x Zn x O alloys. Journal of Materials Science, 2015, 50, 1350-1357.	3.7	17
92	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><mml: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
93	Effect of extended strain fields on point defect phonon scattering in thermoelectric materials. Physical Chemistry Chemical Physics, 2015, 17, 19410-19423.	2.9	56
94	Semiconducting transition metal oxides. Journal of Physics Condensed Matter, 2015, 27, 283203.	1.9	176
95	Non-equilibrium alloying controls optoelectronic properties in Cu2O thin films for photovoltaic absorber applications. Applied Physics Letters, 2015, 106, 123903.	3.2	26
96	Self-regulated growth and tunable properties of CuSbS2 solar absorbers. Solar Energy Materials and Solar Cells, 2015, 132, 499-506.	6.3	125
97	Modeling amorphous thin films: Kinetically limited minimization. Physical Review B, 2014, 90, .	3.3	13
98	Improving electron transport in Ga-doped Zn0.7Mg0.3O, a wide-gap band-edge-energy-tunable transparent conducting oxide. , 2014, , .		0
99	Composition Dependence of the Band Gap and Doping in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Cu</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn><mml:mn mathvariant="normal">O</mml:mi></mml:mrow></mml:math>-Based Alloys as Predicted by an Extension of the Dilute-Defect Model. Physical Review Applied, 2014, 2, .	3.8	18
100	Polymorphism, band-structure, band-lineup, and alloy energetics of the group II oxides and sulfides MgO, ZnO, CdO, MgS, ZnS, CdS. Proceedings of SPIE, 2014, , .	1.0	4
101	Structural and electronic modification of photovoltaic SnS by alloying. Journal of Applied Physics, 2014, 115, .	2.3	30
102	Control of the Electrical Properties in Spinel Oxides by Manipulating the Cation Disorder. Advanced Functional Materials, 2014, 24, 610-618.	16.5	114
103	Enhanced Electron Mobility Due to Dopantâ€Defect Pairing in Conductive ZnMgO. Advanced Functional Materials, 2014, 24, 2875-2882.	16.5	52
104	Assessing capability of semiconductors to split water using ionization potentials and electron affinities only. Physical Chemistry Chemical Physics, 2014, 16, 3706.	2.9	231
105	Non-equilibrium deposition of phase pure Cu2O thin films at reduced growth temperature. APL Materials, 2014, 2, .	4.8	55
106	Defect Tolerant Semiconductors for Solar Energy Conversion. Journal of Physical Chemistry Letters, 2014, 5, 1117-1125.	4.9	318
107	Experimental Characterization of a Theoretically Designed Candidate p-Type Transparent Conducting Oxide: Li-Doped Cr₂MnO₄. Chemistry of Materials, 2014, 26, 4598-4604.	7.1	16
108	Multivalency of Group 15 Dopants in SnO₂. Chemistry of Materials, 2014, 26, 4876-4881.	7.1	11

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109	Control of Doping in Cu₂SnS₃ through Defects and Alloying. Chemistry of Materials, 2014, 26, 4951-4959.	7.1	138
110	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
111	Evaluation of photovoltaic materials within the Cu-Sn-S family. Applied Physics Letters, 2013, 103, .	3.2	120
112	Convergence of density and hybrid functional defect calculations for compound semiconductors. Physical Review B, 2013, 88, .	3.3	100
113	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>. Physical Review B, 2013, 87, .	3.3	169
114	Liâ€Doped Cr₂MnO₄: A New pâ€Type Transparent Conducting Oxide by Computational Materials Design. Advanced Functional Materials, 2013, 23, 5267-5276.	16.5	60
115	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
116	Polymorphic energy ordering of MgO, ZnO, GaN, and MnO within the random phase approximation. Physical Review B, 2013, 87, .	3.3	52
117	Non-equilibrium origin of high electrical conductivity in gallium zinc oxide thin films. Applied Physics Letters, 2013, 103, .	3.2	51
118	Semiconducting 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 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, 2013, 87, .	3.3	75
119	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>: Optoelectronic properties of a conductive spinel oxide. Physical Review B, 2013, 87, .	3.3	73
120	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
121	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
122	Band-structure, optical properties, and defect physics of the photovoltaic semiconductor SnS. Applied Physics Letters, 2012, 100, .	3.2	390
123	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
124	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<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>ZrO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2012, 108, 116403.	8.0	60
125	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:mi></mml:mi></mml:mrow></mml:math>compounds via first-principles thermodynamics. Physical Review B, 2012, 86, .	3.3	46
126	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

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127	Co3O4â€“Co2ZnO4 spinels: The case for a solid solution. Journal of Solid State Chemistry, 2012, 190, 143-149.	3.0	15
128	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/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>. Physical Review B, 2012, 86, .	3.3	40
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