Chris Wolverton

List of Publications by Year
in descending order

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		2538	2883
423	42,029	96	190
papers	citations	h-index	g-index

432	432	432	28439
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ultralow thermal conductivity and high thermoelectric figure of merit in SnSe crystals. Nature, 2014, 508, 373-377.	13.7	3,963
2	Electrical energy storage for transportationâ€”approaching the limits of, and going beyond, lithium-ion batteries. Energy and Environmental Science, 2012, 5, 7854.	15.6	2,086
3	Ultrahigh power factor and thermoelectric performance in hole-doped single-crystal SnSe. Science, 2016, 351, 141-144.	6.0	1,594
4	Materials Design and Discovery with High-Throughput Density Functional Theory: The Open Quantum Materials Database (OQMD). Jom, 2013, 65, 1501-1509.	0.9	1,461
5	The Open Quantum Materials Database (OQMD): assessing the accuracy of DFT formation energies. Npj Computational Materials, 2015, 1, .	3.5	1,200
6	High capacity hydrogenstorage materials: attributes for automotive applications and techniques for materials discovery. Chemical Society Reviews, 2010, 39, 656-675.	18.7	1,008
7	A general-purpose machine learning framework for predicting properties of inorganic materials. Npj Computational Materials, 2016, 2, .	3.5	922
8	All-scale hierarchical thermoelectrics: MgTe in PbTe facilitates valence band convergence and suppresses bipolar thermal transport for high performance. Energy and Environmental Science, 2013, 6, 3346.	15.6	646
9	High Thermoelectric Performance of p-Type SnTe via a Synergistic Band Engineering and Nanostructuring Approach. Journal of the American Chemical Society, 2014, 136, 7006-7017.	6.6	553
10	Combinatorial screening for new materials in unconstrained composition space with machine learning. Physical Review B, 2014, 89, .	1.1	527
11	Non-equilibrium processing leads to record high thermoelectric figure of merit in PbTeâ€“SrTe. Nature Communications, 2016, 7, 12167.	5.8	498
12	Crystal structure and stability of complex precipitate phases in Alâ€“Cuâ€“Mgâ€“(Si) and Alâ€“Znâ€“Mg alloys. Acta Materialia, 2001, 49, 3129-3142.	3.8	394
13	Codoping in SnTe: Enhancement of Thermoelectric Performance through Synergy of Resonance Levels and Band Convergence. Journal of the American Chemical Society, 2015, 137, 5100-5112.	6.6	394
14	Valence Band Modification and High Thermoelectric Performance in SnTe Heavily Alloyed with MnTe. Journal of the American Chemical Society, 2015, 137, 11507-11516.	6.6	371
15	Accelerated discovery of metallic glasses through iteration of machine learning and high-throughput experiments. Science Advances, 2018, 4, eaaq1566.	4.7	354
16	Extraordinary role of Hg in enhancing the thermoelectric performance of p-type SnTe. Energy and Environmental Science, 2015, 8, 267-277.	15.6	347
17	High Thermoelectric Performance via Hierarchical Compositionally Alloyed Nanostructures. Journal of the American Chemical Society, 2013, 135, 7364-7370.	6.6	344
18	Soluteâ€“vacancy binding in aluminum. Acta Materialia, 2007, 55, 5867-5872.	3.8	326

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19	Origin of the High Performance in GeTe-Based Thermoelectric Materials upon Bi₂Te₃ Doping. Journal of the American Chemical Society, 2014, 136, 11412-11419.	6.6	319
20	Raising the Thermoelectric Performance of p-Type PbS with Endotaxial Nanostructuring and Valence-Band Offset Engineering Using CdS and ZnS. Journal of the American Chemical Society, 2012, 134, 16327-16336.	6.6	308
21	Rhombohedral to Cubic Conversion of GeTe via MnTe Alloying Leads to Ultralow Thermal Conductivity, Electronic Band Convergence, and High Thermoelectric Performance. Journal of the American Chemical Society, 2018, 140, 2673-2686.	6.6	307
22	Hydrogen in aluminum: First-principles calculations of structure and thermodynamics. Physical Review B, 2004, 69, .	1.1	300
23	Cu-Au, Ag-Au, Cu-Ag, and Ni-Au intermetallics: First-principles study of temperature-composition phase diagrams and structures. Physical Review B, 1998, 57, 6427-6443.	1.1	271
24	First-principles study of binary bcc alloys using special quasirandom structures. Physical Review B, 2004, 69, .	1.1	266
25	Toward Computational Materials Design: The Impact of Density Functional Theory on Materials Research. MRS Bulletin, 2006, 31, 659-668.	1.7	265
26	High-throughput DFT calculations of formation energy, stability and oxygen vacancy formation energy of ABO3 perovskites. Scientific Data, 2017, 4, 170153.	2.4	259
27	First-Principles Prediction of Thermodynamically Reversible Hydrogen Storage Reactions in the Li-Mg-Ca-B-H System. Journal of the American Chemical Society, 2009, 131, 230-237.	6.6	256
28	Including crystal structure attributes in machine learning models of formation energies via Voronoi tessellations. Physical Review B, 2017, 96, .	1.1	254
29	Multiscale modeling of Î¸â€² precipitation in Alâ€“Cu binary alloys. Acta Materialia, 2004, 52, 2973-2987.	3.8	253
30	First-Principles Prediction of Vacancy Order-Disorder and Intercalation Battery Voltages inLixCoO2. Physical Review Letters, 1998, 81, 606-609.	2.9	252
31	Destabilizing LiBH₄ with a Metal (M = Mg, Al, Ti, V, Cr, or Sc) or Metal Hydride (MH₂ = MgH₂, TiH₂, or CaH₂). Journal of Physical Chemistry C, 2007, 111, 19134-19140.	1.5	246
32	ElemNet: Deep Learning the Chemistry of Materials From Only Elemental Composition. Scientific Reports, 2018, 8, 17593.	1.6	242
33	High thermoelectric performance in Bi_{0.46}Sb_{1.54}Te₃ nanostructured with ZnTe. Energy and Environmental Science, 2018, 11, 1520-1535.	15.6	239
34	First-Principles Calculation of Self-Diffusion Coefficients. Physical Review Letters, 2008, 100, 215901.	2.9	231
35	Phase stability and structure of spinel-based transition aluminas. Physical Review B, 2000, 63, .	1.1	228
36	High ZT in p-Type (PbTe)_{1â€“2x}(PbSe)_x(PbS)_x Thermoelectric Materials. Journal of the American Chemical Society, 2014, 136, 3225-3237.	6.6	228

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37	First Principles Simulations of the Electrochemical Lithiation and Delithiation of Faceted Crystalline Silicon. Journal of the American Chemical Society, 2012, 134, 14362-14374.	6.6	221
38	Firstâ€Principles Determination of Multicomponent Hydride Phase Diagrams: Application to the Liâ€Mgâ€Nâ€H System. Advanced Materials, 2007, 19, 3233-3239.	11.1	217
39	Method for locating low-energy solutions within<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>DFT</mml:mtext><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math> Physical Review B, 2010, 82, .	1.1	215
40	Revealing molecular-level surface redox sites of controllably oxidized black phosphorus nanosheets. Nature Materials, 2019, 18, 156-162.	13.3	215
41	First principles impurity diffusion coefficients. Acta Materialia, 2009, 57, 4102-4108.	3.8	213
42	Computational investigation of half-Heusler compounds for spintronics applications. Physical Review B, 2017, 95, .	1.1	208
43	Recent advances and applications of deep learning methods in materials science. Npj Computational Materials, 2022, 8, .	3.5	207
44	Precipitates in Alâ€“Cu alloys revisited: Atom-probe tomographic experiments and first-principles calculations of compositional evolution and interfacial segregation. Acta Materialia, 2011, 59, 6187-6204.	3.8	206
45	First-principles description of anomalously low lattice thermal conductivity in thermoelectric Cu-Sb-Se ternary semiconductors. Physical Review B, 2012, 85, .	1.1	196
46	Ultrathin Lithium-Ion Conducting Coatings for Increased Interfacial Stability in High Voltage Lithium-Ion Batteries. Chemistry of Materials, 2014, 26, 3128-3134.	3.2	192
47	Materials science with large-scale data and informatics: Unlocking new opportunities. MRS Bulletin, 2016, 41, 399-409.	1.7	192
48	High-Throughput Computational Screening of Perovskites for Thermochemical Water Splitting Applications. Chemistry of Materials, 2016, 28, 5621-5634.	3.2	191
49	Entropically Favored Ordering: The Metallurgy ofAl2CuRevisited. Physical Review Letters, 2001, 86, 5518-5521.	2.9	187
50	Interface and heterostructure design in polyelemental nanoparticles. Science, 2019, 363, 959-964.	6.0	171
51	Atomistic calculations and materials informatics: A review. Current Opinion in Solid State and Materials Science, 2017, 21, 167-176.	5.6	169
52	Ultralow Thermal Conductivity in Full Heusler Semiconductors. Physical Review Letters, 2016, 117, 046602.	2.9	163
53	A machine learning approach for engineering bulk metallic glass alloys. Acta Materialia, 2018, 159, 102-111.	3.8	163
54	Role of silicon in accelerating the nucleation of Al3(Sc,Zr) precipitates in dilute Alâ€“Scâ€“Zr alloys. Acta Materialia, 2012, 60, 4740-4752.	3.8	161

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55	Multiscale Modeling of Precipitate Microstructure Evolution. Physical Review Letters, 2002, 88, 125503.	2.9	160
56	High Thermoelectric Performance in Electron-Doped AgBi₃S₅ with Ultralow Thermal Conductivity. Journal of the American Chemical Society, 2017, 139, 6467-6473.	6.6	160
57	Electrochemistry of Selenium with Sodium and Lithium: Kinetics and Reaction Mechanism. ACS Nano, 2016, 10, 8788-8795.	7.3	155
58	All-Inorganic Halide Perovskites as Potential Thermoelectric Materials: Dynamic Cation off-Centering Induces Ultralow Thermal Conductivity. Journal of the American Chemical Society, 2020, 142, 9553-9563.	6.6	155
59	Performance of the strongly constrained and appropriately normed density functional for solid-state materials. Physical Review Materials, 2018, 2, .	0.9	155
60	First-Principles Prediction of a Ground State Crystal Structure of Magnesium Borohydride. Physical Review Letters, 2008, 100, 135501.	2.9	153
61	Intermediate phases in sodium intercalation into MoS2 nanosheets and their implications for sodium-ion batteries. Nano Energy, 2017, 38, 342-349.	8.2	151
62	High Thermoelectric Performance in SnTeâ€“AgSbTe₂ Alloys from Lattice Softening, Giant Phononâ€“Vacancy Scattering, and Valence Band Convergence. ACS Energy Letters, 2018, 3, 705-712.	8.8	151
63	Highâ€Throughput Computational Screening of New Liâ€ion Battery Anode Materials. Advanced Energy Materials, 2013, 3, 252-262.	10.2	150
64	High-throughput computational design of cathode coatings for Li-ion batteries. Nature Communications, 2016, 7, 13779.	5.8	145
65	Concerted Rattling in CsAg₅Te₃ Leading to Ultralow Thermal Conductivity and High Thermoelectric Performance. Angewandte Chemie - International Edition, 2016, 55, 11431-11436.	7.2	144
66	Virtual aluminum castings: An industrial application of ICME. Jom, 2006, 58, 28-35.	0.9	140
67	Enabling the high capacity of lithium-rich anti-fluorite lithium iron oxide by simultaneous anionic and cationic redox. Nature Energy, 2017, 2, 963-971.	19.8	140
68	Au@MoS₂ Coreâ€“Shell Heterostructures with Strong Lightâ€“Matter Interactions. Nano Letters, 2016, 16, 7696-7702.	4.5	139
69	Developing an improved crystal graph convolutional neural network framework for accelerated materials discovery. Physical Review Materials, 2020, 4, .	0.9	138
70	Thermodynamic stability of Mg-based ternary long-period stacking ordered structures. Acta Materialia, 2014, 68, 325-338.	3.8	134
71	First-principles study of the nucleation and stability of ordered precipitates in ternary Alâ€“Scâ€“Li alloys. Acta Materialia, 2011, 59, 3012-3023.	3.8	133
72	Computational Prediction of High Thermoelectric Performance in Hole Doped Layered GeSe. Chemistry of Materials, 2016, 28, 3218-3226.	3.2	129

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73	Achieving zT > 1 in Inexpensive Zintl Phase Ca₉Zn₄₊_xSb₉ by Phase Boundary Mapping. Advanced Functional Materials, 2017, 27, 1606361.	7.8	129
74	Cation and vacancy ordering inLixCoO2. Physical Review B, 1998, 57, 2242-2252.	1.1	128
75	Role of Sodium Doping in Lead Chalcogenide Thermoelectrics. Journal of the American Chemical Society, 2013, 135, 4624-4627.	6.6	128
76	Thermodynamic guidelines for the prediction of hydrogen storage reactions and their application to destabilized hydride mixtures. Physical Review B, 2007, 76, .	1.1	127
77	Predictions of new <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="italic">AB</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> perovskite compounds by combining machine learning and density functional theory. Physical Review Materials, 2018, 2, .	0.9	127
78	Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure. Physical Review B, 2016, 93, .	1.1	125
79	First-principles theory of vibrational effects on the phase stability of Cu-Au compounds and alloys. Physical Review B, 1998, 58, R5897-R5900.	1.1	123
80	Particlelike Phonon Propagation Dominates Ultralow Lattice Thermal Conductivity in Crystalline <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Tl</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Physical Review Letters, 2020, 124, 065901.	2.9	122
81	Controlling the Intercalation Chemistry to Design High-Performance Dual-Salt Hybrid Rechargeable Batteries. Journal of the American Chemical Society, 2014, 136, 16116-16119.	6.6	120
82	Pd₂Se₃ Monolayer: A Promising Two-Dimensional Thermoelectric Material with Ultralow Lattice Thermal Conductivity and High Power Factor. Chemistry of Materials, 2018, 30, 5639-5647.	3.2	119
83	Soft phonon modes from off-center Ge atoms lead to ultralow thermal conductivity and superior thermoelectric performance in n-type PbSeâ€“GeSe. Energy and Environmental Science, 2018, 11, 3220-3230.	15.6	115
84	First-principles study of soluteâ€“vacancy binding in magnesium. Acta Materialia, 2010, 58, 531-540.	3.8	113
85	Weak Electron Phonon Coupling and Deep Level Impurity for High Thermoelectric Performance Pb_{1â^'}_xGa_xTe. Advanced Energy Materials, 2018, 8, 1800659.	10.2	111
86	First-principles aluminum database: Energetics of binary Al alloys and compounds. Physical Review B, 2006, 73, .	1.1	110
87	Prediction of Li Intercalation and Battery Voltages in Layered vs. Cubic Li x CoO2. Journal of the Electrochemical Society, 1998, 145, 2424-2431.	1.3	109
88	Lithium transport through lithium-ion battery cathode coatings. Journal of Materials Chemistry A, 2015, 3, 17248-17272.	5.2	109
89	Shape regulation of high-index facet nanoparticles by dealloying. Science, 2019, 365, 1159-1163.	6.0	108
90	High Thermoelectric Performance in the New Cubic Semiconductor AgSnSbSe₃ by High-Entropy Engineering. Journal of the American Chemical Society, 2020, 142, 15187-15198.	6.6	108

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91	A hybrid computationalâ€“experimental approach for automated crystal structure solution. Nature Materials, 2013, 12, 123-127.	13.3	107
92	Extraordinary role of Zn in enhancing thermoelectric performance of Ga-doped n-type PbTe. Energy and Environmental Science, 2022, 15, 368-375.	15.6	107
93	First-principles theory of short-range order in size-mismatched metal alloys: Cu-Au, Cu-Ag, and Ni-Au. Physical Review B, 1998, 57, 4332-4348.	1.1	105
94	A valence balanced rule for discovery of 18-electron half-Heuslers with defects. Energy and Environmental Science, 2018, 11, 1480-1488.	15.6	105
95	First-principles thermodynamic framework for the evaluation of thermochemical <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>H</mml:mtext><mml:mn>2</mml:mn></mml:msub><mml:mtext>O</mml:mtext></mml:mrow></mml:math> or <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> materials. Physical Review B, 2009, 80, .	1.1	104
96	van der Waals Interactions in Layered Lithium Cobalt Oxides. Journal of Physical Chemistry C, 2015, 119, 19053-19058.	1.5	103
97	nâ€Type SnSe₂ Orientedâ€Nanoplateâ€Based Pellets for High Thermoelectric Performance. Advanced Energy Materials, 2018, 8, 1702167.	10.2	103
98	Double Half-Heuslers. Joule, 2019, 3, 1226-1238.	11.7	103
99	High-Performance Thermoelectrics from Cellular Nanostructured Sb2Si2Te6. Joule, 2020, 4, 159-175.	11.7	103
100	Lithium Transport in Amorphous Al₂O₃ and AlF₃ for Discovery of Battery Coatings. Journal of Physical Chemistry C, 2013, 117, 8009-8013.	1.5	101
101	First-principles theory of short-range order, electronic excitations, and spin polarization in Ni-V and Pd-V alloys. Physical Review B, 1995, 52, 8813-8828.	1.1	100
102	Morphology Control of Nanostructures: Na-Doped PbTeâ€“PbS System. Nano Letters, 2012, 12, 5979-5984.	4.5	100
103	Thermodynamic Aspects of Cathode Coatings for Lithiumâ€Ion Batteries. Advanced Energy Materials, 2014, 4, 1400690.	10.2	99
104	High Thermoelectric Performance in Polycrystalline SnSe Via Dualâ€Doping with Ag/Na and Nanostructuring With Ag₈SnSe₆. Advanced Energy Materials, 2019, 9, 1803072.	10.2	98
105	Morphological Engineering of Winged Au@MoS₂ Heterostructures for Electrocatalytic Hydrogen Evolution. Nano Letters, 2018, 18, 7104-7110.	4.5	96
106	Electronic-structure methods for materials design. Nature Materials, 2021, 20, 736-749.	13.3	96
107	First-principles prediction of equilibrium precipitate shapes in Al-Cu alloys. Philosophical Magazine Letters, 1999, 79, 683-690.	0.5	93
108	Hydrogen storage in calcium alanate: First-principles thermodynamics and crystal structures. Physical Review B, 2007, 75, .	1.1	93

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109	Predicting Î²â€² precipitate morphology and evolution in Mgâ€“RE alloys using a combination of first-principles calculations and phase-field modeling. Acta Materialia, 2014, 76, 259-271.	3.8	93
110	A fingerprint based metric for measuring similarities of crystalline structures. Journal of Chemical Physics, 2016, 144, 034203.	1.2	93
111	Using the 18-Electron Rule To Understand the Nominal 19-Electron Half-Heusler NbCoSb with Nb Vacancies. Chemistry of Materials, 2017, 29, 1210-1217.	3.2	93
112	Superior Oxygen Reduction Reaction on Phosphorusâ€Doped Carbon Dot/Graphene Aerogel for Allâ€Solidâ€State Flexible Alâ€“Air Batteries. Advanced Energy Materials, 2020, 10, 1902736.	10.2	93
113	High Thermoelectric Performance in Supersaturated Solid Solutions and Nanostructured nâ€Type PbTeâ€“GeTe. Advanced Functional Materials, 2018, 28, 1801617.	7.8	92
114	Incorporating first-principles energetics in computational thermodynamics approaches. Acta Materialia, 2002, 50, 2187-2197.	3.8	91
115	Kinetics and Thermodynamics of H₂O Dissociation on Reduced CeO₂(111). Journal of Physical Chemistry C, 2014, 118, 27402-27414.	1.5	91
116	Systematic Study of Oxygen Vacancy Tunable Transport Properties of Fewâ€Layer MoO_{3â^'}_x Enabled by Vaporâ€Based Synthesis. Advanced Functional Materials, 2017, 27, 1605380.	7.8	91
117	First-principles calculations of Î²â€³-Mg5Si6/Î±-Al interfaces. Acta Materialia, 2007, 55, 5934-5947.	3.8	88
118	Formation of high-strength <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si4.gif" overflow="scroll"><mml:mrow><mml:msup><mml:mrow><mml:mi>Î²</mml:mi></mml:mrow><mml:mrow><mml:mo>â€²</mml:mo></ precipitates in Mgâ€“RE alloys: The role of the Mg/<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si3.gif" overflow="scroll"><mml:mrow><mml:msup><mml:mrow><mml:mi>Î²</mml:mi></mml:mrow><mml:mrow><mml:mo>â€³</mml:mo></	3.8	88
119	Performance of Cluster Expansions of Coverage-Dependent Adsorption of Atomic Oxygen on Pt(111). Journal of Chemical Theory and Computation, 2012, 8, 264-273.	2.3	87
120	All-Scale Hierarchically Structured p-Type PbSe Alloys with High Thermoelectric Performance Enabled by Improved Band Degeneracy. Journal of the American Chemical Society, 2019, 141, 4480-4486.	6.6	87
121	High-throughput computational search for strengthening precipitates in alloys. Acta Materialia, 2016, 102, 125-135.	3.8	83
122	Discordant nature of Cd in GeTe enhances phonon scattering and improves band convergence for high thermoelectric performance. Journal of Materials Chemistry A, 2020, 8, 1193-1204.	5.2	83
123	First-Principles Theory of Competing Order Types, Phase Separation, and Phonon Spectra in Thermoelectric<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>AgPb</mml:mi><mml:mi>m</mml:mi></mml:msub><mml:msub><mml:mi>SbTe</mml:mi><mml:mi><r Physical Review Letters, 2008, 101, 155704.	2.9	82
124	Local environment dependent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mtext>GGA</mml:mtext><mml:mo>+</mml:mo><mml:mi>U</mml:mi></ for accurate thermochemistry of transition metal compounds. Physical Review B, 2014, 90, .	3.7	82
125	Ising-like Description of Structurally Relaxed Ordered and Disordered Alloys. Physical Review Letters, 1995, 75, 3162-3165.	2.9	81
126	Pressure induced thermoelectric enhancement in SnSe crystals. Journal of Materials Chemistry A, 2016, 4, 12073-12079.	5.2	81

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127	Comprehensive Enhancement of Nanostructured Lithium-Ion Battery Cathode Materials via Conformal Graphene Dispersion. Nano Letters, 2017, 17, 2539-2546.	4.5	81
128	Lead-Free Broadband Orange-Emitting Zero-Dimensional Hybrid (PMA)₃InBr₆ with Direct Band Gap. Inorganic Chemistry, 2019, 58, 15602-15609.	1.9	81
129	Material design of high-capacity Li-rich layered-oxide electrodes: Li₂MnO₃ and beyond. Energy and Environmental Science, 2017, 10, 2201-2211.	15.6	80
130	Chemical Insights into PbSeâ€“x%HgSe: High Power Factor and Improved Thermoelectric Performance by Alloying with Discordant Atoms. Journal of the American Chemical Society, 2018, 140, 18115-18123.	6.6	80
131	Na₃Zr₂Si₂PO₁₂: A Stable Na⁺-Ion Solid Electrolyte for Solid-State Batteries. ACS Applied Energy Materials, 2020, 3, 7427-7437.	2.5	77
132	Ab initioprediction of ordered ground-state structures in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>ZrO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms Physical Review B, 2008, 77, .	1.1	76
133	Thermodynamic stability of Coâ€“Alâ€“W L12 Î³â€². Acta Materialia, 2013, 61, 2330-2338.	3.8	76
134	High Figure of Merit in Gallium-Doped Nanostructured n-Type PbTe-xGeTe with Midgap States. Journal of the American Chemical Society, 2019, 141, 16169-16177.	6.6	76
135	Discovery of novel hydrogen storage materials: an atomic scale computational approach. Journal of Physics Condensed Matter, 2008, 20, 064228.	0.7	75
136	Approaching chemical accuracy with density functional calculations: Diatomic energy corrections. Physical Review B, 2013, 87, .	1.1	75
137	First-principles/Phase-field modeling of Î¸â€² precipitation in Al-Cu alloys. Acta Materialia, 2017, 140, 344-354.	3.8	75
138	Effects of anharmonic strain on the phase stability of epitaxial films and superlattices: Applications to noble metals. Physical Review B, 1998, 57, 4816-4828.	1.1	73
139	A combined CALPHAD/first-principles remodeling of the thermodynamics of Alâ€“Sr: unsuspected ground state energies by â€œrounding up the (un)usual suspectsâ€• Acta Materialia, 2004, 52, 2739-2754.	3.8	72
140	Suppressing Manganese Dissolution from Lithium Manganese Oxide Spinel Cathodes with Singleâ€Layer Graphene. Advanced Energy Materials, 2015, 5, 1500646.	10.2	72
141	Network analysis of synthesizable materials discovery. Nature Communications, 2019, 10, 2018.	5.8	72
142	Reaction energetics and crystal structure ofLi4BN3H10from first principles. Physical Review B, 2007, 75, .	1.1	70
143	Predicting the morphologies of Î³Ê¹ precipitates in cobalt-based superalloys. Acta Materialia, 2017, 141, 273-284.	3.8	70
144	Physical factors controlling the observed high-strength precipitate morphology in Mgâ€“rare earth alloys. Acta Materialia, 2014, 65, 240-250.	3.8	69

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145	Computational investigation of inverse Heusler compounds for spintronics applications. Physical Review B, 2018, 98, .	1.1	69
146	Crystal structure and luminescence properties of lead-free metal halides (C₆H₅CH₂NH₃)₃MBr₆ (M = Bi) Tj ET 2 Tq 0 0 0 rg BT /Overl	2.2	69
147	Ab initiodetermination of structural stability in fcc-based transition-metal alloys. Physical Review B, 1993, 48, 726-747.	1.1	68
148	First-principles study of noble gas impurities and defects in UO<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, 2011, 84, .	1.1	68
149	First-principles phase stability, magnetic properties and solubility in aluminumâ€“rare-earth (Alâ€“RE) alloys and compounds. Acta Materialia, 2011, 59, 3659-3666.	3.8	68
150	Dynamic imaging of crystalline defects in lithium-manganese oxide electrodes during electrochemical activation to high voltage. Nature Communications, 2019, 10, 1692.	5.8	68
151	Theoretical prediction of low-energy crystal structures and hydrogen storage energetics inLi2NH. Physical Review B, 2006, 73, .	1.1	67
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