Chris Wolverton

List of Publications by Citations

403 papers	30,817 citations	87 h-index	165 g-index
432 ext. papers	36,418 ext. citations	10.3 avg, IF	7.7 L-index

#	Paper	IF	Citations
403	Ultralow thermal conductivity and high thermoelectric figure of merit in SnSe crystals. *Nature*, **2014**, 508, 373-7	50.4	3074
402	Electrical energy storage for transportation—approaching the limits of, and going beyond, lithium-ion batteries. *Energy and Environmental Science*, **2012**, 5, 7854	35.4	1763
401	Ultrahigh power factor and thermoelectric performance in hole-doped single-crystal SnSe. *Science*, **2016**, 351, 141-4	33.3	1237
400	Materials Design and Discovery with High-Throughput Density Functional Theory: The Open Quantum Materials Database (OQMD). *Jom*, **2013**, 65, 1501-1509	2.1	938
399	High capacity hydrogen storage materials: attributes for automotive applications and techniques for materials discovery. *Chemical Society Reviews*, **2010**, 39, 656-75	58.5	867
398	The Open Quantum Materials Database (OQMD): assessing the accuracy of DFT formation energies. *Npj Computational Materials*, **2015**, 1,	10.9	670
397	A general-purpose machine learning framework for predicting properties of inorganic materials. *Npj Computational Materials*, **2016**, 2,	10.9	558
396	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	35.4	532
395	High thermoelectric performance of p-type SnTe via a synergistic band engineering and nanostructuring approach. *Journal of the American Chemical Society*, **2014**, 136, 7006-17	16.4	425
394	Combinatorial screening for new materials in unconstrained composition space with machine learning. *Physical Review B*, **2014**, 89,	3.3	393
393	Non-equilibrium processing leads to record high thermoelectric figure of merit in PbTe-SrTe. *Nature Communications*, **2016**, 7, 12167	17.4	377
392	Crystal structure and stability of complex precipitate phases in Al–Cu–Mg–(Si) and Al–Zn–Mg alloys. *Acta Materialia*, **2001**, 49, 3129-3142	8.4	334
391	Codoping in SnTe: Enhancement of Thermoelectric Performance through Synergy of Resonance Levels and Band Convergence. *Journal of the American Chemical Society*, **2015**, 137, 5100-12	16.4	310
390	Valence Band Modification and High Thermoelectric Performance in SnTe Heavily Alloyed with MnTe. *Journal of the American Chemical Society*, **2015**, 137, 11507-16	16.4	289
389	High thermoelectric performance via hierarchical compositionally alloyed nanostructures. *Journal of the American Chemical Society*, **2013**, 135, 7364-70	16.4	281
388	Extraordinary role of Hg in enhancing the thermoelectric performance of p-type SnTe. *Energy and Environmental Science*, **2015**, 8, 267-277	35.4	279
387	Solute–vacancy binding in aluminum. *Acta Materialia*, **2007**, 55, 5867-5872	8.4	266

386	Hydrogen in aluminum: First-principles calculations of structure and thermodynamics. *Physical Review B*, **2004**, 69,	3.3	266
385	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, 16327-36	16.4	264
384	Origin of the high performance in GeTe-based thermoelectric materials upon Bi2Te3 doping. *Journal of the American Chemical Society*, **2014**, 136, 11412-9	16.4	259
383	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	3.3	249
382	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, 230-7	16.4	242
381	Accelerated discovery of metallic glasses through iteration of machine learning and high-throughput experiments. *Science Advances*, **2018**, 4, eaaq1566	14.3	237
380	First-principles study of binary bcc alloys using special quasirandom structures. *Physical Review B*, **2004**, 69,	3.3	228
379	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	3.8	227
378	Toward Computational Materials Design: The Impact of Density Functional Theory on Materials Research. *MRS Bulletin*, **2006**, 31, 659-668	3.2	221
377	First-Principles Prediction of Vacancy Order-Disorder and Intercalation Battery Voltages in LixCoO2. *Physical Review Letters*, **1998**, 81, 606-609	7.4	217
376	Multiscale modeling of θ precipitation in Al□u binary alloys. *Acta Materialia*, **2004**, 52, 2973-2987	8.4	209
375	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	16.4	206
374	High ZT in p-type (PbTe)1-2x(PbSe)x(PbS)x thermoelectric materials. *Journal of the American Chemical Society*, **2014**, 136, 3225-37	16.4	198
373	Phase stability and structure of spinel-based transition aluminas. *Physical Review B*, **2000**, 63,	3.3	198
372	First-principles calculation of self-diffusion coefficients. *Physical Review Letters*, **2008**, 100, 215901	7.4	197
371	First principles simulations of the electrochemical lithiation and delithiation of faceted crystalline silicon. *Journal of the American Chemical Society*, **2012**, 134, 14362-74	16.4	192
370	First-Principles Determination of Multicomponent Hydride Phase Diagrams: Application to the Li-Mg-N-H System. *Advanced Materials*, **2007**, 19, 3233-3239	24	191
369	Method for locating low-energy solutions within DFT+U. *Physical Review B*, **2010**, 82,	3.3	187

368	First principles impurity diffusion coefficients. *Acta Materialia*, **2009**, 57, 4102-4108	8.4	184
367	Precipitates in Al–Cu alloys revisited: Atom-probe tomographic experiments and first-principles calculations of compositional evolution and interfacial segregation. *Acta Materialia*, **2011**, 59, 6187-6204	8.4	169
366	Ultrathin Lithium-Ion Conducting Coatings for Increased Interfacial Stability in High Voltage Lithium-Ion Batteries. *Chemistry of Materials*, **2014**, 26, 3128-3134	9.6	164
365	First-principles description of anomalously low lattice thermal conductivity in thermoelectric Cu-Sb-Se ternary semiconductors. *Physical Review B*, **2012**, 85,	3.3	161
364	Entropically favored ordering: the metallurgy of Al(2)Cu revisited. *Physical Review Letters*, **2001**, 86, 5518-21	7.4	160
363	Including crystal structure attributes in machine learning models of formation energies via Voronoi tessellations. *Physical Review B*, **2017**, 96,	3.3	158
362	High thermoelectric performance in Bi0.46Sb1.54Te3 nanostructured with ZnTe. *Energy and Environmental Science*, **2018**, 11, 1520-1535	35.4	155
361	Materials science with large-scale data and informatics: Unlocking new opportunities. *MRS Bulletin*, **2016**, 41, 399-409	3.2	155
360	Revealing molecular-level surface redox sites of controllably oxidized black phosphorus nanosheets. *Nature Materials*, **2019**, 18, 156-162	27	150
359	Multiscale modeling of precipitate microstructure evolution. *Physical Review Letters*, **2002**, 88, 125503	7.4	145
358	High-throughput DFT calculations of formation energy, stability and oxygen vacancy formation energy of ABO perovskites. *Scientific Data*, **2017**, 4, 170153	8.2	144
357	First-principles prediction of a ground state crystal structure of magnesium borohydride. *Physical Review Letters*, **2008**, 100, 135501	7.4	140
356	High-Throughput Computational Screening of Perovskites for Thermochemical Water Splitting Applications. *Chemistry of Materials*, **2016**, 28, 5621-5634	9.6	137
355	Computational investigation of half-Heusler compounds for spintronics applications. *Physical Review B*, **2017**, 95,	3.3	136
354	ElemNet: Deep Learning the Chemistry of Materials From Only Elemental Composition. *Scientific Reports*, **2018**, 8, 17593	4.9	131
353	Atomistic calculations and materials informatics: A review. *Current Opinion in Solid State and Materials Science*, **2017**, 21, 167-176	12	122
352	Intermediate phases in sodium intercalation into MoS2 nanosheets and their implications for sodium-ion batteries. *Nano Energy*, **2017**, 38, 342-349	17.1	119
351	Electrochemistry of Selenium with Sodium and Lithium: Kinetics and Reaction Mechanism. *ACS Nano*, **2016**, 10, 8788-95	16.7	119

350	Role of silicon in accelerating the nucleation of Al3(Sc,Zr) precipitates in dilute Al–Sc–Zr alloys. *Acta Materialia*, **2012**, 60, 4740-4752	8.4	119
349	Virtual aluminum castings: An industrial application of ICME. *Jom*, **2006**, 58, 28-35	2.1	117
348	Interface and heterostructure design in polyelemental nanoparticles. *Science*, **2019**, 363, 959-964	33.3	116
347	High Thermoelectric Performance in Electron-Doped AgBiS with Ultralow Thermal Conductivity. *Journal of the American Chemical Society*, **2017**, 139, 6467-6473	16.4	115
346	High-Throughput Computational Screening of New Li-Ion Battery Anode Materials. *Advanced Energy Materials*, **2013**, 3, 252-262	21.8	115
345	First-principles theory of vibrational effects on the phase stability of Cu-Au compounds and alloys. *Physical Review B*, **1998**, 58, R5897-R5900	3.3	114
344	Thermodynamic guidelines for the prediction of hydrogen storage reactions and their application to destabilized hydride mixtures. *Physical Review B*, **2007**, 76,	3.3	114
343	Cation and vacancy ordering in LixCoO2. *Physical Review B*, **1998**, 57, 2242-2252	3.3	113
342	High-throughput computational design of cathode coatings for Li-ion batteries. *Nature Communications*, **2016**, 7, 13779	17.4	112
341	Au@MoS Core-Shell Heterostructures with Strong Light-Matter Interactions. *Nano Letters*, **2016**, 16, 7696-7702	11.5	111
340	Role of sodium doping in lead chalcogenide thermoelectrics. *Journal of the American Chemical Society*, **2013**, 135, 4624-7	16.4	111
339	Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure. *Physical Review B*, **2016**, 93,	3.3	108
338	First-principles study of the nucleation and stability of ordered precipitates in ternary Al–Sc–Li alloys. *Acta Materialia*, **2011**, 59, 3012-3023	8.4	107
337	Performance of the strongly constrained and appropriately normed density functional for solid-state materials. *Physical Review Materials*, **2018**, 2,	3.2	106
336	Concerted Rattling in CsAg5 Te3 Leading to Ultralow Thermal Conductivity and High Thermoelectric Performance. *Angewandte Chemie - International Edition*, **2016**, 55, 11431-6	16.4	105
335	Thermodynamic stability of Mg-based ternary long-period stacking ordered structures. *Acta Materialia*, **2014**, 68, 325-338	8.4	104
334	Ultralow Thermal Conductivity in Full Heusler Semiconductors. *Physical Review Letters*, **2016**, 117, 046602	7.4	103
333	First-principles aluminum database: Energetics of binary Al alloys and compounds. *Physical Review B*, **2006**, 73,	3.3	103

332	Controlling the intercalation chemistry to design high-performance dual-salt hybrid rechargeable batteries. *Journal of the American Chemical Society*, **2014**, 136, 16116-9	16.4	99
331	Achieving zT > 1 in Inexpensive Zintl Phase Ca9Zn4+xSb9 by Phase Boundary Mapping. *Advanced Functional Materials*, **2017**, 27, 1606361	15.6	98
330	A machine learning approach for engineering bulk metallic glass alloys. *Acta Materialia*, **2018**, 159, 102-111	8.4	97
329	A hybrid computational-experimental approach for automated crystal structure solution. *Nature Materials*, **2013**, 12, 123-7	27	96
328	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	3.3	92
327	Prediction of Li Intercalation and Battery Voltages in Layered vs. Cubic Li x CoO2. *Journal of the Electrochemical Society*, **1998**, 145, 2424-2431	3.9	92
326	First-principles study of solute□vacancy binding in magnesium. *Acta Materialia*, **2010**, 58, 531-540	8.4	91
325	Computational Prediction of High Thermoelectric Performance in Hole Doped Layered GeSe. *Chemistry of Materials*, **2016**, 28, 3218-3226	9.6	91
324	High Thermoelectric Performance in SnTe□AgSbTe2 Alloys from Lattice Softening, Giant Phonon□Vacancy Scattering, and Valence Band Convergence. *ACS Energy Letters*, **2018**, 3, 705-712	20.1	90
323	Enabling the high capacity of lithium-rich anti-fluorite lithium iron oxide by simultaneous anionic and cationic redox. *Nature Energy*, **2017**, 2, 963-971	62.3	90
322	Morphology control of nanostructures: Na-doped PbTe-PbS system. *Nano Letters*, **2012**, 12, 5979-84	11.5	90
321	First-principles thermodynamic framework for the evaluation of thermochemical H2O- or CO2-splitting materials. *Physical Review B*, **2009**, 80,	3.3	88
320	Hydrogen storage in calcium alanate: First-principles thermodynamics and crystal structures. *Physical Review B*, **2007**, 75,	3.3	88
319	First-principles prediction of equilibrium precipitate shapes in Al-Cu alloys. *Philosophical Magazine Letters*, **1999**, 79, 683-690	1	88
318	Predictions of new ABO3 perovskite compounds by combining machine learning and density functional theory. *Physical Review Materials*, **2018**, 2,	3.2	88
317	Lithium Transport in Amorphous Al2O3 and AlF3 for Discovery of Battery Coatings. *Journal of Physical Chemistry C*, **2013**, 117, 8009-8013	3.8	87
316	Thermodynamic Aspects of Cathode Coatings for Lithium-Ion Batteries. *Advanced Energy Materials*, **2014**, 4, 1400690	21.8	84
315	Incorporating first-principles energetics in computational thermodynamics approaches. *Acta Materialia*, **2002**, 50, 2187-2197	8.4	83

314	Lithium transport through lithium-ion battery cathode coatings. *Journal of Materials Chemistry A*, **2015**, 3, 17248-17272	13	82
313	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	3.3	82
312	van der Waals Interactions in Layered Lithium Cobalt Oxides. *Journal of Physical Chemistry C*, **2015**, 119, 19053-19058	3.8	80
311	Performance of Cluster Expansions of Coverage-Dependent Adsorption of Atomic Oxygen on Pt(111). *Journal of Chemical Theory and Computation*, **2012**, 8, 264-73	6.4	79
310	n-Type SnSe2 Oriented-Nanoplate-Based Pellets for High Thermoelectric Performance. *Advanced Energy Materials*, **2018**, 8, 1702167	21.8	76
309	Soft phonon modes from off-center Ge atoms lead to ultralow thermal conductivity and superior thermoelectric performance in n-type PbSe□GeSe. *Energy and Environmental Science*, **2018**, 11, 3220-3230	35.4	75
308	A fingerprint based metric for measuring similarities of crystalline structures. *Journal of Chemical Physics*, **2016**, 144, 034203	3.9	75
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306	Predicting β′ precipitate morphology and evolution in MgRE alloys using a combination of first-principles calculations and phase-field modeling. *Acta Materialia*, **2014**, 76, 259-271	8.4	74
305	First-principles theory of competing order types, phase separation, and phonon spectra in thermoelectric AgPbmSbTe(m+2) alloys. *Physical Review Letters*, **2008**, 101, 155704	7.4	73
304	Morphological Engineering of Winged Au@MoS Heterostructures for Electrocatalytic Hydrogen Evolution. *Nano Letters*, **2018**, 18, 7104-7110	11.5	71
303	High Thermoelectric Performance in Supersaturated Solid Solutions and Nanostructured n-Type PbTe□GeTe. *Advanced Functional Materials*, **2018**, 28, 1801617	15.6	69
302	Ising-like description of structurally relaxed ordered and disordered alloys. *Physical Review Letters*, **1995**, 75, 3162-3165	7.4	69
301	A valence balanced rule for discovery of 18-electron half-Heuslers with defects. *Energy and Environmental Science*, **2018**, 11, 1480-1488	35.4	68
300	High-throughput computational search for strengthening precipitates in alloys. *Acta Materialia*, **2016**, 102, 125-135	8.4	67
299	Local environment dependent GGA+U method for accurate thermochemistry of transition metal compounds. *Physical Review B*, **2014**, 90,	3.3	67
298	Reaction energetics and crystal structure of Li4BN3H10 from first principles. *Physical Review B*, **2007**, 75,	3.3	67
297	Comprehensive Enhancement of Nanostructured Lithium-Ion Battery Cathode Materials via Conformal Graphene Dispersion. *Nano Letters*, **2017**, 17, 2539-2546	11.5	66

296	Systematic Study of Oxygen Vacancy Tunable Transport Properties of Few-Layer MoO3 Enabled by Vapor-Based Synthesis. *Advanced Functional Materials*, **2017**, 27, 1605380	15.6	66
295	First-principles calculations of -Mg5Si6/Al interfaces. *Acta Materialia*, **2007**, 55, 5934-5947	8.4	66
294	Formation of high-strength precipitates in MgRE alloys: The role of the Mg/ interfacial instability. *Acta Materialia*, **2015**, 83, 75-83	8.4	65
293	Ab initio prediction of ordered ground-state structures in ZrO2-Y2O3. *Physical Review B*, **2008**, 77,	3.3	65
292	Theoretical prediction of low-energy crystal structures and hydrogen storage energetics in Li2NH. *Physical Review B*, **2006**, 73,	3.3	65
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290	Ab initio determination of structural stability in fcc-based transition-metal alloys. *Physical Review B*, **1993**, 48, 726-747	3.3	65
289	Pressure induced thermoelectric enhancement in SnSe crystals. *Journal of Materials Chemistry A*, **2016**, 4, 12073-12079	13	65
288	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	16.4	64
287	Pd2Se3 Monolayer: A Promising Two-Dimensional Thermoelectric Material with Ultralow Lattice Thermal Conductivity and High Power Factor. *Chemistry of Materials*, **2018**, 30, 5639-5647	9.6	64
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283	A combined CALPHAD/first-principles remodeling of the thermodynamics of AlSr: unsuspected ground state energies by ounding up the (un)usual suspects *Acta Materialia*, **2004**, 52, 2739-2754	8.4	63
282	Shape regulation of high-index facet nanoparticles by dealloying. *Science*, **2019**, 365, 1159-1163	33.3	62
281	Superior Oxygen Reduction Reaction on Phosphorus-Doped Carbon Dot/Graphene Aerogel for All-Solid-State Flexible Al Air Batteries. *Advanced Energy Materials*, **2020**, 10, 1902736	21.8	62
280	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	16.4	62
279	First-principles study of noble gas impurities and defects in UO2. *Physical Review B*, **2011**, 84,	3.3	61

278	Approaching chemical accuracy with density functional calculations: Diatomic energy corrections. *Physical Review B*, **2013**, 87,	3.3	60
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276	Suppressing Manganese Dissolution from Lithium Manganese Oxide Spinel Cathodes with Single-Layer Graphene. *Advanced Energy Materials*, **2015**, 5, 1500646	21.8	60
275	Chemical Insights into PbSe- x%HgSe: High Power Factor and Improved Thermoelectric Performance by Alloying with Discordant Atoms. *Journal of the American Chemical Society*, **2018**, 140, 18115-18123	16.4	60
274	Using the 18-Electron Rule To Understand the Nominal 19-Electron Half-Heusler NbCoSb with Nb Vacancies. *Chemistry of Materials*, **2017**, 29, 1210-1217	9.6	59
273	First-principles phase stability, magnetic properties and solubility in aluminum□are-earth (Al□RE) alloys and compounds. *Acta Materialia*, **2011**, 59, 3659-3666	8.4	59
272	Kinetics and Thermodynamics of H2O Dissociation on Reduced CeO2(111). *Journal of Physical Chemistry C*, **2014**, 118, 27402-27414	3.8	58
271	Physical factors controlling the observed high-strength precipitate morphology in Mg□are earth alloys. *Acta Materialia*, **2014**, 65, 240-250	8.4	55
270	High-Performance Thermoelectrics from Cellular Nanostructured Sb2Si2Te6. *Joule*, **2020**, 4, 159-175	27.8	55
269	Surface phase diagram and stability of (001) and (111) LiMn2O4 spinel oxides. *Physical Review B*, **2015**, 92,	3.3	54
268	Predicting metastable phase boundaries in Al□Cu alloys from first-principles calculations of free energies: The role of atomic vibrations. *Europhysics Letters*, **2006**, 73, 719-725	1.6	54
267	Kinetically-Driven Phase Transformation during Lithiation in Copper Sulfide Nanoflakes. *Nano Letters*, **2017**, 17, 5726-5733	11.5	53
266	Prediction of New Stable Compounds and Promising Thermoelectrics in the Cu□Sb□Se System. *Chemistry of Materials*, **2014**, 26, 3427-3435	9.6	52
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260	Enhancement of Thermoelectric Performance for n-Type PbS through Synergy of Gap State and Fermi Level Pinning. *Journal of the American Chemical Society*, **2019**, 141, 6403-6412	16.4	48
259	Ni-Au: A testing ground for theories of phase stability. *Computational Materials Science*, **1997**, 8, 107-121	3.2	48
258	Revealing the Conversion Mechanism of Transition Metal Oxide Electrodes during Lithiation from First-Principles. *Chemistry of Materials*, **2017**, 29, 9011-9022	9.6	46
257	Double Half-Heuslers. *Joule*, **2019**, 3, 1226-1238	27.8	46
256	Enhanced Density-of-States Effective Mass and Strained Endotaxial Nanostructures in Sb-Doped PbCdTe Thermoelectric Alloys. *ACS Applied Materials & Interfaces*, **2019**, 11, 9197-9204	9.5	46
255	First-principles determination of crystal structures, phase stability, and reaction thermodynamics in the Li-Mg-Al-H hydrogen storage system. *Physical Review B*, **2009**, 79,	3.3	46
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252	High Figure of Merit in Gallium-Doped Nanostructured n-Type PbTe-GeTe with Midgap States. *Journal of the American Chemical Society*, **2019**, 141, 16169-16177	16.4	44
251	Out-of-Plane Mechanical Properties of 2D Hybrid Organic-Inorganic Perovskites by Nanoindentation. *ACS Applied Materials & Interfaces*, **2018**, 10, 22167-22173	9.5	44
250	Implications of coverage-dependent O adsorption for catalytic NO oxidation on the late transition metals. *Catalysis Science and Technology*, **2014**, 4, 4356-4365	5.5	44
249	Solute□vacancy binding of the rare earths in magnesium from first principles. *Acta Materialia*, **2012**, 60, 5151-5159	8.4	44
248	Predicting the morphologies of □ precipitates in cobalt-based superalloys. *Acta Materialia*, **2017**, 141, 273-284	8.4	43
247	Thermodynamic stability of Mg□□n long-period stacking ordered structures. *Scripta Materialia*, **2012**, 67, 798-801	5.6	43
246	Short- and long-range order of the binary Madelung lattice. *Physical Review B*, **1995**, 51, 6876-6891	3.3	43
245	Developing an improved crystal graph convolutional neural network framework for accelerated materials discovery. *Physical Review Materials*, **2020**, 4,	3.2	43
244	Interplay of cation and anion redox in LiMnO cathode material and prediction of improved Li(Mn,M)O electrodes for Li-ion batteries. *Science Advances*, **2018**, 4, eaao6754	14.3	43
243	Diffusion coefficients of transition metals in fcc cobalt. *Acta Materialia*, **2017**, 132, 467-478	8.4	42

242	Lead-Free Broadband Orange-Emitting Zero-Dimensional Hybrid (PMA)InBr with Direct Band Gap. *Inorganic Chemistry*, **2019**, 58, 15602-15609	5.1	42
241	High Thermoelectric Performance in PbSe□NaSbSe2 Alloys from Valence Band Convergence and Low Thermal Conductivity. *Advanced Energy Materials*, **2019**, 9, 1901377	21.8	42
240	Particlelike Phonon Propagation Dominates Ultralow Lattice Thermal Conductivity in Crystalline Tl_{3}VSe_{4}. *Physical Review Letters*, **2020**, 124, 065901	7.4	41
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237	Network analysis of synthesizable materials discovery. *Nature Communications*, **2019**, 10, 2018	17.4	40
236	Theoretical prediction of different decomposition paths for Ca(BH4)2 and Mg(BH4)2. *Physical Review B*, **2010**, 82,	3.3	40
235	High Thermoelectric Performance in the New Cubic Semiconductor AgSnSbSe by High-Entropy Engineering. *Journal of the American Chemical Society*, **2020**, 142, 15187-15198	16.4	40
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232	Coherent and incoherent phase stabilities of thermoelectric rocksalt IV-VI semiconductor alloys. *Physical Review B*, **2012**, 86,	3.3	38
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230	Machine-learning-accelerated high-throughput materials screening: Discovery of novel quaternary Heusler compounds. *Physical Review Materials*, **2018**, 2,	3.2	38
229	Discovery of Calcium-Metal Alloy Anodes for Reversible Ca-Ion Batteries. *Advanced Energy Materials* , **2019**, 9, 1802994	21.8	38
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