Dane D Morgan

List of Publications by Citations

324 papers	16,613 citations	57 h-index	121 g-index
369 ext. papers	18,664 ext. citations	5.5 avg, IF	6.87 L-index

#	Paper	IF	Citations
324	First-principles study of native point defects in ZnO. *Physical Review B*, **2000**, 61, 15019-15027	3.3	1454
323	Instability of Pt□ Electrocatalysts in Proton Exchange Membrane Fuel Cells. *Journal of the Electrochemical Society*, **2005**, 152, A2256	3.9	1170
322	Li Conductivity in Li[sub x]MPO[sub 4] (M = Mn, Fe, Co, Ni) Olivine Materials. *Electrochemical and Solid-State Letters*, **2004**, 7, A30		924
321	Instability of Supported Platinum Nanoparticles in Low-Temperature Fuel Cells. *Topics in Catalysis*, **2007**, 46, 285-305	2.3	731
320	First-principles prediction of redox potentials in transition-metal compounds with LDA+U. *Physical Review B*, **2004**, 70,	3.3	705
319	AFLOW: An automatic framework for high-throughput materials discovery. *Computational Materials Science*, **2012**, 58, 218-226	3.2	581
318	Prediction of solid oxide fuel cell cathode activity with first-principles descriptors. *Energy and Environmental Science*, **2011**, 4, 3966	35.4	345
317	Ab initio energetics of LaBO3(001) (B=Mn, Fe, Co, and Ni) for solid oxide fuel cell cathodes. *Physical Review B*, **2009**, 80,	3.3	331
316	Predicting crystal structure by merging data mining with quantum mechanics. *Nature Materials*, **2006**, 5, 641-6	27	329
315	Predicting crystal structures with data mining of quantum calculations. *Physical Review Letters*, **2003**, 91, 135503	7.4	317
314	The electronic structure and band gap of LiFePO4 and LiMnPO4. *Solid State Communications*, **2004**, 132, 181-186	1.6	307
313	Accuracy of ab initio methods in predicting the crystal structures of metals: A review of 80 binary alloys. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2005**, 29, 163-211	1.9	266
312	Surface strontium enrichment on highly active perovskites for oxygen electrocatalysis in solid oxide fuel cells. *Energy and Environmental Science*, **2012**, 5, 6081	35.4	257
311	Pt nanoparticle stability in PEM fuel cells: influence of particle size distribution and crossover hydrogen. *Energy and Environmental Science*, **2009**, 2, 865	35.4	218
310	Nondilute diffusion from first principles: Li diffusion in LixTiS2. *Physical Review B*, **2008**, 78,	3.3	197
309	New frontiers for the materials genome initiative. *Npj Computational Materials*, **2019**, 5,	10.9	171
308	Electrochemical modeling of intercalation processes with phase field models. *Electrochimica Acta*, **2004**, 49, 4691-4699	6.7	169

307	First-principles study of the stability and electronic structure of metal hydrides. *Physical Review B*, **2002**, 66,	3.3	167
306	Origins of Large Voltage Hysteresis in High-Energy-Density Metal Fluoride Lithium-Ion Battery Conversion Electrodes. *Journal of the American Chemical Society*, **2016**, 138, 2838-48	16.4	166
305	Experimental and Computational Study of the Structure and Electrochemical Properties of LixM2(PO4)3 Compounds with the Monoclinic and Rhombohedral Structure. *Chemistry of Materials*, **2002**, 14, 4684-4693	9.6	157
304	Phase Stability of Nickel Hydroxides and Oxyhydroxides. *Journal of the Electrochemical Society*, **2006**, 153, A210	3.9	148
303	Phase separation in LixFePO4 induced by correlation effects. *Physical Review B*, **2004**, 69,	3.3	147
302	Phase transformations and volume changes in spinel LixMn2O4. *Solid State Ionics*, **2000**, 135, 21-32	3.3	140
301	Dynamic layer rearrangement during growth of layered oxide films by molecular beam epitaxy. *Nature Materials*, **2014**, 13, 879-83	27	117
300	High-throughput computational design of cathode coatings for Li-ion batteries. *Nature Communications*, **2016**, 7, 13779	17.4	112
299	Ab initio-based diffusion theory and tracer diffusion in Ni□r and Ni□e alloys. *Journal of Nuclear Materials*, **2010**, 405, 216-234	3.3	109
298	Nanometre-thick single-crystalline nanosheets grown at the water-air interface. *Nature Communications*, **2016**, 7, 10444	17.4	100
297	Tuning perovskite oxides by strain: Electronic structure, properties, and functions in (electro)catalysis and ferroelectricity. *Materials Today*, **2019**, 31, 100-118	21.8	98
296	Phase Diagram of Mg Insertion into Chevrel Phases, MgxMo6T8 (T = S, Se). 1. Crystal Structure of the Sulfides. *Chemistry of Materials*, **2006**, 18, 5492-5503	9.6	98
295	Assessment of radiation-induced segregation mechanisms in austenitic and ferritic□hartensitic alloys. *Journal of Nuclear Materials*, **2011**, 411, 41-50	3.3	97
294	Predicting the thermodynamic stability of perovskite oxides using machine learning models. *Computational Materials Science*, **2018**, 150, 454-463	3.2	95
293	High-throughput and data mining with ab initio methods. *Measurement Science and Technology*, **2005**, 16, 296-301	2	95
292	Ab-initio based modeling of diffusion in dilute bcc Fe□i and Fe□r alloys and implications for radiation induced segregation. *Journal of Nuclear Materials*, **2011**, 411, 1-14	3.3	93
291	Material Discovery and Design Principles for Stable, High Activity Perovskite Cathodes for Solid Oxide Fuel Cells. *Advanced Energy Materials*, **2018**, 8, 1702708	21.8	83
290	Atomic Layer Deposited MgO: A Lower Overpotential Coating for Li[NiMnCo]O Cathode. *ACS Applied Materials & Interfaces*, **2017**, 9, 11231-11239	9.5	82

289	Lithium transport through lithium-ion battery cathode coatings. *Journal of Materials Chemistry A*, **2015**, 3, 17248-17272	13	82
288	Ag diffusion in cubic silicon carbide. *Journal of Nuclear Materials*, **2011**, 408, 257-271	3.3	82
287	Embedded-atom-method study of structural, thermodynamic, and atomic-transport properties of liquid Ni-Al alloys. *Physical Review B*, **1999**, 59, 14271-14281	3.3	81
286	Effects of grain size and grain boundaries on defect production in nanocrystalline 3C□SiC. *Acta Materialia*, **2010**, 58, 2843-2853	8.4	79
285	Epitaxial Strain-Induced Chemical Ordering in La0.5Sr0.5CoO3□Films on SrTiO3. *Chemistry of Materials*, **2011**, 23, 984-988	9.6	76
284	Understanding and Controlling the Work Function of Perovskite Oxides Using Density Functional Theory. *Advanced Functional Materials*, **2016**, 26, 5471-5482	15.6	75
283	Ab initio GGA+U study of oxygen evolution and oxygen reduction electrocatalysis on the (001) surfaces of lanthanum transition metal perovskites LaBO□(B = Cr, Mn, Fe, Co and Ni). *Physical Chemistry Chemical Physics*, **2015**, 17, 21643-63	3.6	74
282	High-throughput ab-initio dilute solute diffusion database. *Scientific Data*, **2016**, 3, 160054	8.2	71
281	First-principles investigation of the cooperative Jahn-Teller effect for octahedrally coordinated transition-metal ions. *Physical Review B*, **2001**, 63,	3.3	71
280	Density Functional Theory Study of Ferrihydrite and Related Fe-Oxyhydroxides. *Chemistry of Materials*, **2009**, 21, 5727-5742	9.6	66
279	First-principles alloy theory in oxides. *Modelling and Simulation in Materials Science and Engineering*, **2000**, 8, 311-321	2	66
278	Catalytic Activity and Stability of Oxides: The Role of Near-Surface Atomic Structures and Compositions. *Accounts of Chemical Research*, **2016**, 49, 966-73	24.3	65
277	Ab initio study of the composition dependence of the pressure-induced spin crossover in perovskite (Mg1□,Fex)SiO3. *Earth and Planetary Science Letters*, **2008**, 265, 535-545	5.3	63
276	Anomalous Interface and Surface Strontium Segregation in (La1-ySry)2CoO4□/La1-xSrxCoO3-□ Heterostructured Thin Films. *Journal of Physical Chemistry Letters*, **2014**, 5, 1027-34	6.4	62
275	Correlation and relativistic effects in U metal and U-Zr alloy: Validation of ab initio approaches. *Physical Review B*, **2013**, 88,	3.3	62
274	Strain effects on oxygen migration in perovskites. *Physical Chemistry Chemical Physics*, **2015**, 17, 2715-21	3.6	61
273	First-principles molecular dynamics modeling of the LiCl□KCl molten salt system. *Computational Materials Science*, **2014**, 83, 362-370	3.2	61
272	Opportunities and Challenges for Machine Learning in Materials Science. *Annual Review of Materials Research*, **2020**, 50, 71-103	12.8	60

271	Ab initio study of the composition dependence of the pressure-induced spin transition in the (Mg1−x,Fex)O system. *Geophysical Research Letters*, **2006**, 33,	4.9	59
270	Experimental and computational study of the structure and electrochemical properties of monoclinic LixM2(PO4)3 compounds. *Journal of Power Sources*, **2003**, 119-121, 755-759	8.9	58
269	Elemental vacancy diffusion database from high-throughput first-principles calculations for fcc and hcp structures. *New Journal of Physics*, **2014**, 16, 015018	2.9	57
268	Stable p-type conduction from Sb-decorated head-to-head basal plane inversion domain boundaries in ZnO nanowires. *Nano Letters*, **2012**, 12, 1311-6	11.5	57
267	Assessing Correlations of Perovskite Catalytic Performance with Electronic Structure Descriptors. *Chemistry of Materials*, **2019**, 31, 785-797	9.6	57
266	Multi-technique characterization of the precipitates in thermally aged and neutron irradiated Fe-Cu and Fe-Cu-Mn model alloys: Atom probe tomography reconstruction implications. *Acta Materialia*, **2018**, 146, 237-252	8.4	56
265	Automated defect analysis in electron microscopic images. *Npj Computational Materials*, **2018**, 4,	10.9	54
264	In situ anomalous small-angle X-ray scattering studies of platinum nanoparticle fuel cell electrocatalyst degradation. *Journal of the American Chemical Society*, **2012**, 134, 14823-33	16.4	54
263	First Principles Study of H-insertion in MnO2. *Journal of Solid State Chemistry*, **2002**, 166, 91-103	3.3	54
262	Application of Pt Nanoparticle Dissolution and Oxidation Modeling to Understanding Degradation in PEM Fuel Cells. *Journal of the Electrochemical Society*, **2012**, 159, B578-B591	3.9	53
261	Oxygen surface exchange kinetics and stability of (La,Sr)2CoO4±δ/La1−xSrxMO3−δ (M = Co and Fe) hetero-interfaces at intermediate temperatures. *Journal of Materials Chemistry A*, **2015**, 3, 2144-2157	13	52
260	Electronic and magnetic structures of the postperovskite-type Fe2O3 and implications for planetary magnetic records and deep interiors. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 5508-12	11.5	52
259	Thermodynamic and kinetic modeling of Mn-Ni-Si precipitates in low-Cu reactor pressure vessel steels. *Acta Materialia*, **2017**, 138, 10-26	8.4	51
258	Cation interdiffusion model for enhanced oxygen kinetics at oxide heterostructure interfaces. *Physical Chemistry Chemical Physics*, **2012**, 14, 2606-16	3.6	51
257	Report from the third workshop on future directions of solid-state chemistry: The status of solid-state chemistry and its impact in the physical sciences. *Progress in Solid State Chemistry*, **2008**, 36, 1-133	8	51
256	First-principles study of the structure of stoichiometric and Mn-deficient MnO2. *Journal of Solid State Chemistry*, **2003**, 173, 462-475	3.3	51
255	Kinetics of Oxygen Surface Exchange on Epitaxial Ruddlesden-Popper Phases and Correlations to First-Principles Descriptors. *Journal of Physical Chemistry Letters*, **2016**, 7, 244-9	6.4	50
254	Thermodynamics of spinel LixTiO2 from first principles. *Chemical Physics*, **2005**, 317, 130-136	2.3	50

253	Dependence on grain boundary structure of radiation induced segregation in a 9wt.% Cr model ferritic/martensitic steel. *Journal of Nuclear Materials*, **2013**, 435, 172-180	3.3	49
252	Mössbauer modeling to interpret the spin state of iron in (Mg,Fe)SiO3 perovskite. *Geophysical Research Letters*, **2009**, 36, n/a-n/a	4.9	49
251	Vibrational spectra in ordered and disordered Ni3Al. *Physical Review B*, **1997**, 56, R5705-R5708	3.3	49
250	Factors controlling oxygen migration barriers in perovskites. *Solid State Ionics*, **2016**, 296, 71-77	3.3	48
249	First-principles molecular dynamics modeling of the molten fluoride salt with Cr solute. *Journal of Nuclear Materials*, **2014**, 449, 148-157	3.3	48
248	Thermodynamic modeling of the U□r system □A revisit. *Journal of Nuclear Materials*, **2013**, 443, 331-341	3.3	48
247	Tuning the Spin State in LaCoO Thin Films for Enhanced High-Temperature Oxygen Electrocatalysis. *Journal of Physical Chemistry Letters*, **2013**, 4, 2493-2499	6.4	48
246	Ab initio and empirical defect modeling of LaMnO(3□□)for solid oxide fuel cell cathodes. *Physical Chemistry Chemical Physics*, **2012**, 14, 290-302	3.6	48
245	Ab Initio Modeling of Electrolyte Molecule Ethylene Carbonate Decomposition Reaction on Li(Ni,Mn,Co)O Cathode Surface. *ACS Applied Materials & Interfaces*, **2017**, 9, 20545-20553	9.5	47
244	First principles study of Li diffusion in I-Li2NiO2 structure. *Physical Review B*, **2009**, 79,	3.3	47
243	Atomic Layer Deposition of Al2O3-Ga2O3 Alloy Coatings for Li[Ni0.5Mn0.3Co0.2]O2 Cathode to Improve Rate Performance in Li-Ion Battery. *ACS Applied Materials & Interfaces*, **2016**, 8, 10572-80	9.5	45
242	Evolution of small defect clusters in ion-irradiated 3C-SiC: Combined cluster dynamics modeling and experimental study. *Acta Materialia*, **2017**, 125, 377-389	8.4	43
241	Thermodynamics and Hysteresis of Oxide Formation and Removal on Platinum (111) Surfaces. *Journal of Physical Chemistry C*, **2012**, 116, 9942-9946	3.8	43
240	Ab initio study of the strain dependent thermodynamics of Bi doping in GaAs. *Physical Review B*, **2012**, 86,	3.3	42
239	Factors controlling surface oxygen exchange in oxides. *Nature Communications*, **2019**, 10, 1346	17.4	41
238	Pt Catalyst Degradation in Aqueous and Fuel Cell Environments studied via In-Operando Anomalous Small-Angle X-ray Scattering. *Electrochimica Acta*, **2015**, 173, 223-234	6.7	41
237	An ab initio study of Ti□□O nanocluster energetics in nanostructured ferritic alloys. *Acta Materialia* , **2012**, 60, 935-947	8.4	41
236	Ab initio study of the effects of thin CsI coatings on the work function of graphite cathodes. *Applied Physics Letters*, **2007**, 91, 144102	3.4	41

235	Data-Mining-Driven Quantum Mechanics for the Prediction of Structure. *MRS Bulletin*, **2006**, 31, 981-985	3.2	41
234	Effect of Grain Boundary Stresses on Sink Strength. *Materials Research Letters*, **2014**, 2, 100-106	7.4	40
233	Diffusion of Ag along Σ grain boundaries in 3C-SiC. *Physical Review B*, **2011**, 84,	3.3	40
232	Ab initio based rate theory model of radiation induced amorphization in βSiC. *Journal of Nuclear Materials*, **2011**, 414, 431-439	3.3	39
231	Thermodynamics and kinetics of core-shell versus appendage co-precipitation morphologies: An example in the Fe-Cu-Mn-Ni-Si system. *Acta Materialia*, **2018**, 157, 298-306	8.4	38
230	Energy barriers for point-defect reactions in 3C-SiC. *Physical Review B*, **2013**, 88,	3.3	38
229	Cluster dynamics modeling of Mn-Ni-Si precipitates in ferritic-martensitic steel under irradiation. *Journal of Nuclear Materials*, **2018**, 498, 83-88	3.3	37
228	Stability of ferrous-iron-rich bridgmanite under reducing midmantle conditions. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 6468-6473	11.5	37
227	Experimental and ab initio study of enhanced resistance to amorphization of nanocrystalline silicon carbide under electron irradiation. *Journal of Nuclear Materials*, **2014**, 445, 181-189	3.3	37
226	Ab initio investigation of barium-scandium-oxygen coatings on tungsten for electron emitting cathodes. *Physical Review B*, **2010**, 81,	3.3	37
225	Oxygen Point Defect Chemistry in Ruddlesden-Popper Oxides (La1-xSrx)2MO4±δ (M = Co, Ni, Cu). *Journal of Physical Chemistry Letters*, **2016**, 7, 1939-44	6.4	37
224	Ultra-fast evaluation of protein energies directly from sequence. *PLoS Computational Biology*, **2006**, 2, e63	5	36
223	Thermodynamic and kinetic modeling of oxide precipitation in nanostructured ferritic alloys. *Acta Materialia*, **2015**, 91, 340-354	8.4	35
222	Work function and surface stability of tungsten-based thermionic electron emission cathodes. *APL Materials*, **2017**, 5, 116105	5.7	35
221	Robust FCC solute diffusion predictions from ab-initio machine learning methods. *Computational Materials Science*, **2017**, 134, 160-165	3.2	34
220	Materials Discovery of Stable and Nontoxic Halide Perovskite Materials for High-Efficiency Solar Cells. *Advanced Functional Materials*, **2019**, 29, 1804354	15.6	34
219	Strontium influence on the oxygen electrocatalysis of La2−xSrxNiO4±δ (0.0 ≤ x ≤ 1.0) thin films. *Journal of Materials Chemistry A*, **2014**, 2, 6480-6487	13	34
218	Frontiers in Thermionic Cathode Research. *IEEE Transactions on Electron Devices*, **2018**, 65, 2061-2071	2.9	33

217	Redox condition in molten salts and solute behavior: A first-principles molecular dynamics study. *Journal of Nuclear Materials*, **2015**, 465, 224-235	3.3	33
216	Characterization of microstructure and property evolution in advanced cladding and duct: Materials exposed to high dose and elevated temperature. *Journal of Materials Research*, **2015**, 30, 1246-1274	2.5	32
215	Flux effects in precipitation under irradiation □Simulation of Fe-Cr alloys. *Acta Materialia*, **2019**, 164, 586-601	8.4	32
214	Enhanced Oxygen Surface Exchange Kinetics and Stability on Epitaxial La0.8Sr0.2CoO3□Thin Films by La0.8Sr0.2MnO3□Decoration. *Journal of Physical Chemistry C*, **2014**, 118, 14326-14334	3.8	31
213	Coarsening of Pt Nanoparticles in Proton Exchange Membrane Fuel Cells upon Potential Cycling. *ECS Transactions*, **2006**, 1, 185-195	1	31
212	Strain control of oxygen kinetics in the Ruddlesden-Popper oxide LaSrCuO. *Nature Communications*, **2018**, 9, 92	17.4	30
211	Ab initio defect energetics of perovskite (001) surfaces for solid oxide fuel cells: A comparative study of LaMnO3 versus SrTiO3 and LaAlO3. *Physical Review B*, **2015**, 91,	3.3	30
210	Grain boundary character dependence of radiation-induced segregation in a model Ni□Cr alloy. *Journal of Materials Research*, **2015**, 30, 1290-1299	2.5	29
209	Precipitation in Fe-Cu and Fe-Cu-Mn model alloys under irradiation: Dose rate effects. *Acta Materialia*, **2018**, 157, 72-82	8.4	29
208	Ab initio study of point defect structures and energetics in ZrC. *Journal of Applied Physics*, **2010**, 107, 053521	2.5	29
207	Ab initio molecular dynamics simulation of interstitial diffusion in Ni□Cr alloys and implications for radiation induced segregation. *Journal of Nuclear Materials*, **2014**, 449, 225-233	3.3	28
206	Massive interfacial reconstruction at misfit dislocations in metal/oxide interfaces. *Scientific Reports*, **2014**, 4, 6533	4.9	27
205	Thermodynamic models of low-temperature Mn-Ni-Si precipitation in reactor pressure vessel steels. *MRS Communications*, **2014**, 4, 101-105	2.7	27
204	Prediction of concrete coefficient of thermal expansion and other properties using machine learning. *Construction and Building Materials*, **2019**, 220, 587-595	6.7	26
203	Phase Separation Tendencies of Aluminum-Doped Transition-Metal Oxides (LiAl1 □x M x O 2) in the □ - NaFeO2 Crystal Structure. *Journal of the Electrochemical Society*, **1999**, 146, 4335-4338	3.9	26
202	Stretching Epitaxial La0.6Sr0.4CoO3□for Fast Oxygen Reduction. *Journal of Physical Chemistry C*, **2017**, 121, 25651-25658	3.8	25
201	Genetic algorithm optimization of defect clusters in crystalline materials. *Computational Materials Science*, **2015**, 98, 234-244	3.2	25
200	Amorphization driven by defect-induced mechanical instability. *Physical Review Letters*, **2013**, 111, 155501	7.4	25

199	Spin state of iron in Fe3O4 magnetite and h-Fe3O4. *Physical Review B*, **2013**, 87,	3.3	25
198	H and Al Solid-State NMR Study of the Local Environments in Al-Doped 2-Line Ferrihydrite, Goethite, and Lepidocrocite. *Chemistry of Materials*, **2015**, 27, 3966-3978	9.6	25
197	Growth Trajectories and Coarsening Mechanisms of Metal Nanoparticle Electrocatalysts. *ChemCatChem*, **2012**, 4, 766-770	5.2	25
196	Stable interstitial dopant□acancy complexes in ZnO. *Physical Review B*, **2012**, 85,	3.3	25
195	Optimizing AlF3 atomic layer deposition using trimethylaluminum and TaF5: Application to high voltage Li-ion battery cathodes. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **2016**, 34, 031503	2.9	25
194	Spatially resolved mapping of oxygen reduction/evolution reaction on solid-oxide fuel cell cathodes with sub-10 nm resolution. *ACS Nano*, **2013**, 7, 3808-14	16.7	24
193	The MAterials Simulation Toolkit (MAST) for atomistic modeling of defects and diffusion. *Computational Materials Science*, **2017**, 126, 90-102	3.2	24
192	Integrated modeling of second phase precipitation in cold-worked 316 stainless steels under irradiation. *Acta Materialia*, **2017**, 130, 94-110	8.4	23
191	Joint Experimental and Computational O and H Solid State NMR Study of BaInO(OH) Structure and Dynamics. *Chemistry of Materials*, **2015**, 27, 3861-3873	9.6	23
190	Local strain effect on the band gap engineering of graphene by a first-principles study. *Applied Physics Letters*, **2015**, 106, 053113	3.4	23
189	Thermodynamics of Al-substitution in Fe-oxyhydroxides. *Geochimica Et Cosmochimica Acta*, **2013**, 120, 514-530	5.5	23
188	Carbon tri-interstitial defect: A model for the DII center. *Physical Review B*, **2012**, 86,	3.3	23
187	Atomistic modeling of As diffusion in ZnO. *Physical Review B*, **2012**, 85,	3.3	23
186	Ab initio investigation of the surface properties of dispenser B-type and scandate thermionic emission cathodes. *Applied Physics Letters*, **2009**, 94, 184102	3.4	23
185	First-principles study of magnetism in spinel MnO2. *Physical Review B*, **2003**, 67,	3.3	23
184	First-principles investigation on diffusion mechanism of alloying elements in dilute Zr alloys. *Acta Materialia*, **2018**, 154, 161-171	8.4	22
183	Role of recombination kinetics and grain size in radiation-induced amorphization. *Physical Review B*, **2012**, 86,	3.3	22
182	Radiation-induced segregation in a ceramic. *Nature Materials*, **2020**, 19, 992-998	27	22

181	Thermal diffusion boron doping of single-crystal natural diamond. *Journal of Applied Physics*, **2016**, 119, 205703	2.5	22
180	Ag diffusion in SiC high-energy grain boundaries: Kinetic Monte Carlo study with first-principle calculations. *Computational Materials Science*, **2016**, 121, 248-257	3.2	22
179	Strain effects on oxygen vacancy formation energy in perovskites. *Solid State Ionics*, **2017**, 311, 105-117	3.3	21
178	Atomistic modeling of the order□disorder phase transformation in the Ni2Cr model alloy. *Acta Materialia*, **2014**, 81, 258-271	8.4	21
177	Ab initio study of structurally bound water at cation vacancy sites in Fe- and Al-oxyhydroxide materials. *Geochimica Et Cosmochimica Acta*, **2013**, 114, 94-111	5.5	21
176	GaAs1□□PyBiz, an alternative reduced band gap alloy system lattice-matched to GaAs. *Applied Physics Letters*, **2014**, 105, 111101	3.4	21
175	Shape Dependence of Pressure-Induced Phase Transition in CdS Semiconductor Nanocrystals. *Journal of the American Chemical Society*, **2020**, 142, 6505-6510	16.4	20
174	Microstructural Evolution of Type 304 and 316 Stainless Steels Under Neutron Irradiation at LWR Relevant Conditions. *Jom*, **2016**, 68, 517-529	2.1	20
173	Error assessment and optimal cross-validation approaches in machine learning applied to impurity diffusion. *Computational Materials Science*, **2019**, 169, 109075	3.2	20
172	On the Elevated Temperature Thermal Stability of Nanoscale Mn-Ni-Si Precipitates Formed at Lower Temperature in Highly Irradiated Reactor Pressure Vessel Steels. *Scientific Reports*, **2019**, 9, 9587	4.9	20
171	In-Operando Anomalous Small-Angle X-Ray Scattering Investigation of Pt3Co Catalyst Degradation in Aqueous and Fuel Cell Environments. *Journal of the Electrochemical Society*, **2015**, 162, F1487-F1497	3.9	20
170	Automatic construction, implementation and assessment of Pettifor maps. *Journal of Physics Condensed Matter*, **2003**, 15, 4361-4369	1.8	20
169	Integrated Computational and Experimental Structure Refinement for Nanoparticles. *ACS Nano*, **2016**, 10, 4031-8	16.7	20
168	Understanding and reducing deleterious defects in the metastable alloy GaAsBi. *NPG Asia Materials* , **2017**, 9, e345-e345	10.3	19
167	Modeling radiation induced segregation in Ni□r model alloys from first principles. *Journal of Nuclear Materials*, **2012**, 425, 8-15	3.3	19
166	Accelerated atomistic simulation study on the stability and mobility of carbon tri-interstitial cluster in cubic SiC. *Computational Materials Science*, **2014**, 89, 182-188	3.2	19
165	First Principles Investigation of Oxygen Vacancies in Columbite MNb2O6 (M = Mn, Fe, Co, Ni, Cu)□ *Chemistry of Materials*, **2010**, 22, 906-913	9.6	19
164	Radiation interaction with tilt grain boundaries in □SiC. *Journal of Applied Physics*, **2012**, 111, 054918	2.5	19

163	Spin transitions in the FexMn1−xS2 system. *Physical Review B*, **2006**, 73,	3.3	19
162	Polarity-driven oxygen vacancy formation in ultrathin LaNiO3 films on SrTiO3. *Physical Review Materials*, **2017**, 1,	3.2	19
161	Massive Vacancy Concentration Yields Strong Room-Temperature Ferromagnetism in Two-Dimensional ZnO. *Nano Letters*, **2019**, 19, 7085-7092	11.5	18
160	Defect kinetics and resistance to amorphization in zirconium carbide. *Journal of Nuclear Materials*, **2015**, 457, 343-351	3.3	18
159	Intrinsic defects and conduction characteristics of Sc2O3 in thermionic cathode systems. *Physical Review B*, **2012**, 86,	3.3	18
158	Coarse-graining protein energetics in sequence variables. *Physical Review Letters*, **2005**, 95, 148103	7.4	18
157	Factors Controlling Oxygen Interstitial Diffusion in the Ruddlesden−Popper Oxide La2−xSrxNiO4+δ *Chemistry of Materials*, **2018**, 30, 7166-7177	9.6	18
156	Structures and stabilities of small carbon interstitial clusters in cubic silicon carbide. *Acta Materialia*, **2014**, 62, 162-172	8.4	17
155	Cs diffusion in cubic silicon carbide. *Journal of Nuclear Materials*, **2012**, 421, 89-96	3.3	17
154	A review of fission product sorption in carbon structures. *Journal of Nuclear Materials*, **2012**, 426, 254-267	3.3	17
153	Ab initio Defect Energetics in LaBO3 Perovskite Solid Oxide Fuel Cell Materials. *ECS Transactions*, **2009**, 25, 2761-2767	1	17
152	Effects of spin transition on diffusion of Fe2+ in ferropericlase in Earth's lower mantle. *Physical Review B*, **2011**, 84,	3.3	17
151	Local environment effects in the vibrational properties of disordered alloys: An embedded-atom method study of Ni3Al and Cu3Au. *Journal of Phase Equilibria and Diffusion*, **1998**, 19, 559-567		17
150	Enhancement of oxygen surface exchange on epitaxial La0.6Sr0.4Co0.2Fe0.8O3-δ thin films using advanced heterostructured oxide interface engineering. *MRS Communications*, **2016**, 6, 204-209	2.7	17
149	Counterintuitive Reconstruction of the Polar O-Terminated ZnO Surface with Zinc Vacancies and Hydrogen. *Journal of Physical Chemistry Letters*, **2016**, 7, 4483-4487	6.4	16
148	Electron Emission Energy Barriers and Stability of Sc2O3 with Adsorbed Ba and BaO. *Journal of Physical Chemistry C*, **2014**, 118, 19742-19758	3.8	16
147	Vibrational thermodynamics: coupling of chemical order and size effects. *Modelling and Simulation in Materials Science and Engineering*, **2000**, 8, 295-309	2	16
146	Iron partitioning between ferropericlase and bridgmanite in the Earth's lower mantle. *Journal of Geophysical Research: Solid Earth*, **2017**, 122, 1074-1087	3.6	15

145	Effect of Nonuniform Emission on Miram Curves. *IEEE Transactions on Plasma Science*, **2020**, 48, 146-155	1.3	15
144	Increased stability of CuZrAl metallic glasses prepared by physical vapor deposition. *Journal of Alloys and Compounds*, **2017**, 728, 1110-1115	5.7	15
143	Prediction of Surface Oxygen Vacancy Concentrations of (La1-xSrx)MnO3. *ECS Transactions*, **2009**, 25, 2769-2774	1	15
142	CuMnNiSi precipitate evolution in irradiated reactor pressure vessel steels: Integrated Cluster Dynamics and experiments. *Acta Materialia*, **2019**, 180, 199-217	8.4	15
141	Origin of Fe3+ in Fe-containing, Al-free mantle silicate perovskite. *Earth and Planetary Science Letters*, **2015**, 409, 319-328	5.3	14
140	Modeling Deep Burn TRISO particle nuclear fuel. *Journal of Nuclear Materials*, **2012**, 430, 181-189	3.3	14
139	Corrosion of Si, C, and SiC in molten salt. *Corrosion Science*, **2019**, 146, 1-9	6.8	14
138	Kinetic Monte Carlo simulation of the effective diffusivity in grain boundary networks. *Computational Materials Science*, **2014**, 93, 36-45	3.2	13
137	Experimental investigation and thermodynamic modeling of the NiAlRu ternary system. *Acta Materialia*, **2009**, 57, 202-212	8.4	13
136	Modeling of phase stability of the fcc phases in the NiAl system using the cluster/site approximation method coupling with first-principles calculations. *Acta Materialia*, **2008**, 56, 2576-2584	8.4	13
135	Grain boundary diffusion of Ag through polycrystalline SiC in TRISO fuel particles. *Journal of Nuclear Materials*, **2015**, 467, 332-340	3.3	12
134	The Materials Simulation Toolkit for Machine learning (MAST-ML): An automated open source toolkit to accelerate data-driven materials research. *Computational Materials Science*, **2020**, 176, 109544	3.2	12
133	Role of pre-existing point defects on primary damage production and amorphization in silicon carbide (SiC). *Nuclear Instruments & Methods in Physics Research B*, **2018**, 414, 45-60	1.2	12
132	Simulated spatial and temporal dependence of chromium concentration in pure Fe and Fe 14%Cr under high dpa ion irradiation. *Journal of Nuclear Materials*, **2016**, 479, 23-35	3.3	12
131	A-Site Diffusion in La1 SrxMnO3: Ab Initio and Kinetic Monte Carlo Calculations. *Journal of the Electrochemical Society*, **2013**, 160, F877-F882	3.9	12
130	Surface chemical analysis and ab initio investigations of CsI coated C fiber cathodes for high power microwave sources. *Journal of Applied Physics*, **2010**, 107, 044903	2.5	12
129	Impact of substitutional and interstitial carbon defects on lattice parameters in MgB2. *Journal of Applied Physics*, **2010**, 107, 023902	2.5	12
128	Ab initio prediction of threshold displacement energies in ZrC. *Journal of Nuclear Materials*, **2016**, 471, 214-219	3.3	11

127	Evidence for cascade overlap and grain boundary enhanced amorphization in silicon carbide irradiated with Kr ions. *Acta Materialia*, **2015**, 99, 7-15	8.4	11
126	Local Dielectric Breakdown Path along c-Axis Planar Boundaries in Cr2O3 Thin Films. *Advanced Materials Interfaces*, **2017**, 4, 1700172	4.6	11
125	Ab initio and thermodynamic modelling of alloying effects on activity of sacrificial aluminium anodes. *Corrosion Science*, **2011**, 53, 1724-1731	6.8	11
124	Embedded atom method calculations of vibrational thermodynamic properties of ordered and disordered Ni3Al. *Computational Materials Science*, **1998**, 10, 411-415	3.2	11
123	First-principles studies on molecular beam epitaxy growth of GaAs1□Bix. *Physical Review B*, **2015**, 92,	3.3	10
122	First-principles calculation aided thermodynamic modeling of the Mo□e system. *Intermetallics*, **2010**, 18, 574-581	3.5	10
121	Observations of defect structure evolution in proton and Ni ion irradiated Ni-Cr binary alloys. *Journal of Nuclear Materials*, **2016**, 479, 48-58	3.3	10
120	Valleyite: A new magnetic mineral with the sodalite-type structure. *American Mineralogist*, **2019**, 104, 1238-1245	2.9	9
119	Effect of carbon ion irradiation on Ag diffusion in SiC. *Journal of Nuclear Materials*, **2016**, 471, 220-232	3.3	9
118	Thermodynamic evaluation of the Np□r system using CALPHAD and ab initio methods. *Journal of Nuclear Materials*, **2014**, 452, 569-577	3.3	9
117	Diffusion-limited reactions in spherical cavities. *Journal of Chemical Physics*, **1992**, 96, 8840-8852	3.9	9
116	Optimization of self-interstitial clusters in 3C-SiC with genetic algorithm. *Journal of Nuclear Materials*, **2017**, 492, 62-73	3.3	8
115	Continuum model for hydrogen pickup in zirconium alloys of LWR fuel cladding. *Journal of Applied Physics*, **2017**, 121, 135101	2.5	8
114	Density-Functional-Theory Modeling of Cation Diffusion in Bulk La1□SrxMnO3□□(x=0.0□0.25) for Solid-Oxide Fuel-Cell Cathodes. *Physical Review Applied*, **2017**, 8,	4.3	8
113	Exploring effective charge in electromigration using machine learning. *MRS Communications*, **2019**, 9, 567-575	2.7	8
112	Simulation of Cu precipitation in Fe-Cu dilute alloys with cluster mobility. *Materials and Design*, **2020**, 191, 108574	8.1	8
111	Cs and Ag co-incorporation in cubic silicon carbide. *Journal of Nuclear Materials*, **2013**, 439, 65-71	3.3	8
110	Ab initio energetics of charge compensating point defects: A case study on MgO. *Computational Materials Science*, **2013**, 73, 41-55	3.2	8

109	Effect of anomalous compressibility on Fe diffusion in ferropericlase throughout the spin crossover in the lower mantle. *Earth and Planetary Science Letters*, **2013**, 362, 1-5	5.3	8
108	Thermodynamic modeling of the CrPt binary system using the cluster/site approximation coupling with first-principles energetics calculation. *Acta Materialia*, **2008**, 56, 5796-5803	8.4	8
107	Combined ab initio and empirical model of the thermal conductivity of uranium, uranium-zirconium, and uranium-molybdenum. *Physical Review Materials*, **2018**, 2,	3.2	8
106	Understanding the interplay of surface structure and work function in oxides: A case study on SrTiO3. *APL Materials*, **2020**, 8, 071110	5.7	8
105	Impact of Nonuniform Thermionic Emission on the Transition Behavior Between Temperature-and Space-Charge-Limited Emission. *IEEE Transactions on Electron Devices*, **2021**, 68, 3576-3581	2.9	8
104	Radiation-induced mobility of small defect clusters in covalent materials. *Physical Review B*, **2016**, 94,	3.3	8
103	Development of an Electrochemical Oxygen Sensor for Liquid Sodium Using a Yttria Stabilized Zirconia Electrolyte. *Journal of the Electrochemical Society*, **2017**, 164, B10-B22	3.9	7
102	Assessing Graph-based Deep Learning Models for Predicting Flash Point. *Molecular Informatics*, **2020**, 39, e1900101	3.8	7
101	A kinetic lattice Monte Carlo study of post-irradiation annealing of model reactor pressure vessel steels. *Journal of Nuclear Materials*, **2019**, 524, 312-322	3.3	7
100	Joint experimental and computational 17O solid state NMR study of Brownmillerite Ba2In2O5. *Physical Chemistry Chemical Physics*, **2014**, 16, 2597-606	3.6	7
99	First-principles study of Cs and Sr sorption on carbon structures. *Journal of Applied Physics*, **2012**, 111, 094912	2.5	7
98	Machine learning in nuclear materials research. *Current Opinion in Solid State and Materials Science*, **2022**, 26, 100975	12	7
97	Mechanisms of bulk and surface diffusion in metallic glasses determined from molecular dynamics simulations. *Acta Materialia*, **2021**, 209, 116794	8.4	7
96	A deep learning based automatic defect analysis framework for In-situ TEM ion irradiations. *Computational Materials Science*, **2021**, 197, 110560	3.2	7
95	Strain-compensated GaAs1−yPy/GaAs1−xBix/GaAs1−yPyquantum wells for laser applications. *Semiconductor Science and Technology*, **2015**, 30, 094011	1.8	6
94	Assessing Concentration Dependence of FCC Metal Alloy Diffusion Coefficients Using Kinetic Monte Carlo. *Journal of Phase Equilibria and Diffusion*, **2010**, 31, 250-259	1	6
93	Data Mining in Materials Development **2005**, 395-421		6
92	Fast Surface Dynamics on a Metallic Glass Nanowire. *ACS Nano*, **2021**,	16.7	6

91	CALPHAD modeling and ab initio calculations of the Np-U-Zr system. *Computational Materials Science*, **2018**, 143, 505-514	3.2	6
90	Nanoscale Voltage Enhancement at Cathode Interfaces in Li-Ion Batteries. *Chemistry of Materials*, **2017**, 29, 1218-1229	9.6	5
89	An Unexpected Role of H During SiC Corrosion in Water. *Journal of Physical Chemistry C*, **2020**, 124, 9394-9400	3.7	5
88	Reply to "Comment on "Correlation and relativistic effects in U metal and U-Zr alloy: Validation of ab initio approaches"" *Physical Review B*, **2016**, 93,	3.3	5
87	Diffusion of transition metals in periclase by experiment and first-principles, with implications for core–mantle equilibration during metal percolation. *Earth and Planetary Science Letters*, **2012**, 357-358, 42-53	5.3	5
86	Oxide Formation and Removal on Pt Surfaces Under Potential Cycled Conditions. *ECS Transactions*, **2009**, 25, 583-592	1	5
85	Thermodynamic modeling of the Cr–Ir binary system using the cluster/site approximation (CSA) coupling with first-principles energetic calculation. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2009**, 33, 420-424	1.9	5
84	Electronic Structure-Based Descriptors for Oxide Properties and Functions.. *Accounts of Chemical Research*, **2022**,	24.3	5
83	Factors correlating to enhanced surface diffusion in metallic glasses. *Journal of Chemical Physics*, **2021**, 154, 104502	3.9	5
82	First-principles predictions of electronic properties of GaAs1-x-yPyBix and GaAs1-x-yPyBix-based heterojunctions. *Applied Physics Letters*, **2016**, 109, 112104	3.4	5
81	Multi defect detection and analysis of electron microscopy images with deep learning. *Computational Materials Science*, **2021**, 199, 110576	3.2	5
80	The O-O Bonding and Hydrogen Storage in the Pyrite-type PtO. *Inorganic Chemistry*, **2019**, 58, 8300-8307	5.1	4
79	Comment on "Thermal vacancies in random alloys in the single-site mean-field approximation" *Physical Review B*, **2020**, 101,	3.3	4
78	Data and Supplemental information for predicting the thermodynamic stability of perovskite oxides using machine learning models. *Data in Brief*, **2018**, 19, 261-263	1.2	4
77	PEMFC Nanoparticle Catalyst Dealloying from Kinetic Monte Carlo Simulations. *ECS Transactions*, **2013**, 50, 1643-1649	1	4
76	Strain Effects on Defect Chemistry in Epitaxial Perovskite Thin Films for Solid Oxide Fuel Cells. *ECS Transactions*, **2011**, 35, 2113-2118	1	4
75	Crystal structure effect of ferromagnetic electrode on tunneling magnetoresistance. *Acta Materialia*, **2008**, 56, 1491-1495	8.4	4
74	MAST-SEY: MAterial Simulation Toolkit for Secondary Electron Yield. A monte carlo approach to secondary electron emission based on complex dielectric functions. *Computational Materials Science*, **2021**, 193, 110281	3.2	4

73	StructOpt: A modular materials structure optimization suite incorporating experimental data and simulated energies. *Computational Materials Science*, **2019**, 160, 1-8	3.2	4
72	Surface Diffusion Is Controlled by Bulk Fragility across All Glass Types.. *Physical Review Letters*, **2022**, 128, 075501	7.4	4
71	Fast approximate STEM image simulations from a machine learning model. *Advanced Structural and Chemical Imaging*, **2019**, 5,	3.9	3
70	DFT-based prediction of fission product sorption on carbon structures under O2 ingress conditions. *Journal of Nuclear Materials*, **2013**, 437, 389-400	3.3	3
69	Experimental and Simulation Insight on the Transport of Silver Fission Product in SiC **2008**,		3
68	A Drastic Influence of Point Defects on Phase Stability in MnO2. *Materials Research Society Symposia Proceedings*, **2002**, 755, 1		3
67	The incommensurately modulated structures of volcanic plagioclase: displacement, ordering and phase transition. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2019**, 75, 643-656	1.8	3
66	Graph network based deep learning of bandgaps. *Journal of Chemical Physics*, **2021**, 155, 154702	3.9	3
65	Microalloying effect in ternary Al-Sm-X (X□=□Ag, Au, Cu) metallic glasses studied by ab initio molecular dynamics. *Computational Materials Science*, **2020**, 185, 109958	3.2	3
64	Deciphering water-solid reactions during hydrothermal corrosion of SiC. *Acta Materialia*, **2021**, 209, 116803	8.4	3
63	Response to letter □lectron correlation and relativity of the 5f electrons in the U Zr alloy system□ *Journal of Nuclear Materials*, **2016**, 476, 110-112	3.3	3
62	Work Function Trends and New Low-Work-Function Boride and Nitride Materials for Electron Emission Applications. *Journal of Physical Chemistry C*, **2021**, 125, 17400-17410	3.8	3
61	Cs diffusion in SiC high-energy grain boundaries. *Journal of Applied Physics*, **2017**, 122, 105901	2.5	2
60	Identification and Quantification of Boron Dopant Sites in Antiferromagnetic Cr2O3 Films by Electron Energy Loss Spectroscopy. *Microscopy and Microanalysis*, **2017**, 23, 1584-1585	0.5	2
59	Ab initio energetics for modeling phase stability of the Np-U system. *Journal of Nuclear Materials*, **2016**, 479, 260-270	3.3	2
58	Transition state redox during dynamical processes in semiconductors and insulators. *NPG Asia Materials*, **2018**, 10, 45-51	10.3	2
57	Effects of confinements on morphology of InxGa1□As thin film grown on sub-micron patterned GaAs substrate: Elastoplastic phase field model. *Journal of Applied Physics*, **2014**, 116, 114313	2.5	2
56	Bayesian Statistical Model for Imaging of Single La Vacancies in LaMnO3. *Microscopy and Microanalysis*, **2017**, 23, 1572-1573	0.5	2

55	Effect of tetragonal lattice distortion of Co70Fe30 on the tunneling magnetoresistance of AlO x based magnetic tunnel junction. *Applied Physics A: Materials Science and Processing*, **2009**, 97, 73-77	2.6	2
54	Data Mining Approach to Ab-Initio Prediction of Crystal Structure. *Materials Research Society Symposia Proceedings*, **2003**, 804, 305		2
53	The incommensurately modulated structures of low-temperature labradorite feldspars: a single-crystal X-ray and neutron diffraction study. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2020**, 76, 93-107	1.8	2
52	Thermodynamic stability analysis of Bi-containing III-V quaternary alloys and the effect of epitaxial strain. *Journal of Physics and Chemistry of Solids*, **2020**, 138, 109245	3.9	2
51	Evaluation of radiomics and machine learning in identification of aggressive tumor features in renal cell carcinoma (RCC). *Abdominal Radiology*, **2021**, 46, 4278-4288	3	2
50	Development and Deployment of Automated Machine Learning Detection in Electron Microcopy Experiments. *Microscopy and Microanalysis*, **2021**, 27, 2136-2137	0.5	2
49	Three-Dimensional Imaging of Single La Vacancies in LaMnO 3. *Microscopy and Microanalysis*, **2016**, 22, 902-903	0.5	2
48	Discovery and engineering of low work function perovskite materials. *Journal of Materials Chemistry C*, **2021**, 9, 12778-12790	7.1	2
47	Iron valence and partitioning between post-perovskite and ferropericlase in the Earth□s lowermost mantle. *Physics of the Earth and Planetary Interiors*, **2018**, 282, 110-116	2.3	2
46	Exploration of characteristic temperature contributions to metallic glass forming ability. *Computational Materials Science*, **2021**, 196, 110494	3.2	2
45	X-Ray Diffraction and Electron Microscopy Studies of the Size Effects on Pressure-Induced Phase Transitions in CdS Nanocrystals. *MRS Advances*, **2020**, 5, 2447-2455	0.7	1
44	A first-principles and experimental study of helium diffusion in periclase MgO. *Physics and Chemistry of Minerals*, **2018**, 45, 641-654	1.6	1
43	Catalytic Activity of (001)-AO and BO2 Surfaces of Transition Metal Perovskites: Case of LaCrO3. *ECS Transactions*, **2014**, 58, 1-8	1	1
42	Density Functional Theory Modeling of A-site Cation Diffusion in Bulk LaMnO3□for Solid Oxide Fuel Cell Cathodes. *ECS Transactions*, **2017**, 78, 2797-2806	1	1
41	High-throughput computational screening for low work function perovskite electron emitters **2017** ,		1
40	Ab initio model of intrinsic defects in Sc2O3 for thermionic cathode systems **2012**,		1
39	17.2: Ab initio models of dispenser B-type, scandate, and alloy cathode surfaces **2010**,		1
38	Surface chemical analysis of cesium-iodide (CsI) coated carbon (C) fibers and thin films for field emission applications **2009**,		1

37	Ab Initio Study of Oxygen-Vacancy Ordering in Oxygen Conducting Ba2In2O5. *Materials Research Society Symposia Proceedings*, **2006**, 972, 1		1
36	Semi-adsorption-controlled growth window for half-Heusler FeVSb epitaxial films. *Physical Review Materials*, **2020**, 4,	3.2	1
35	Understanding the Formation Energy of Transition Metal Hydrides. *Materials Research Society Symposia Proceedings*, **2002**, 730, 1		1
34	Modified band alignment method to obtain hybrid functional accuracy from standard DFT: Application to defects in highly mismatched III-V:Bi alloys. *Physical Review Materials*, **2021**, 5,	3.2	1
33	A combined ab-initio and empirical model for thermal conductivity of concentrated metal alloys with the focus on binary uranium alloys. *Materialia*, **2021**, 15, 100990	3.2	1
32	A Statistical Method for Emulation of Computer Models With Invariance-Preserving Properties, With Application to Structural Energy Prediction. *Journal of the American Statistical Association*, **2020**, 115, 1798-1811	2.8	1
31	An ab-initio based semi-empirical thermal conductivity model for multiphase uranium-zirconium alloys. *Journal of Nuclear Materials*, **2021**, 553, 153044	3.3	1
30	Molecular simulation-derived features for machine learning predictions of metal glass forming ability. *Computational Materials Science*, **2021**, 199, 110728	3.2	1
29	Performance and limitations of deep learning semantic segmentation of multiple defects in transmission electron micrographs. *Cell Reports Physical Science*, **2022**, 100876	6.1	1
28	Dopant binding with vacancies and helium in metal hydrides. *Journal of Nuclear Materials*, **2021**, 559, 153437	3.3	0
27	Machine learning principles applied to CT radiomics to predict mucinous pancreatic cysts. *Abdominal Radiology*, **2021**, 1	3	0
26	First principles inelastic mean free paths coupled with Monte Carlo simulation of secondary electron yield of Cu-Ni, Cu-Zn, and Mo-Li. *Journal of Applied Physics*, **2021**, 129, 175105	2.5	0
25	Combined ab-initio and empirical model for irradiated metal alloys with a focus on uranium alloy fuel thermal conductivity. *Journal of Nuclear Materials*, **2021**, 549, 152891	3.3	0
24	4D-STEM Determination of Atomic Structure of Amorphous Materials for Renewable Energy Applications. *Microscopy and Microanalysis*, **2021**, 27, 396-398	0.5	0
23	Molecular dynamic characteristic temperatures for predicting metallic glass forming ability. *Computational Materials Science*, **2022**, 201, 110877	3.2	0
22	Machine learning for impurity charge-state transition levels in semiconductors from elemental properties using multi-fidelity datasets.. *Journal of Chemical Physics*, **2022**, 156, 114110	3.9	0
21	Unconventional Highly Active and Stable Oxygen Reduction Catalysts Informed by Computational Design Strategies. *Advanced Energy Materials*,2201203	21.8	0
20	Exposing New Atomic-scale Information about Materials by Improving the Quality and Quantifiability of Aberration-corrected STEM Data **2016**, 495-496		

19	Nanoparticle Structure from Genetic Algorithm Refinement Against Quantitative STEM Data **2016**, 521-522	
18	Discovery of New Minerals of Luogufengite and Valleyite Using Synchrotron X-ray Diffraction and Transmission Electron Microscopy. *Microscopy and Microanalysis*, **2020**, 26, 494-495	0.5
17	Density Functional Theory Study of the Gas Phase and Surface Reaction Kinetics for the MOVPE Growth of GaAsBi. *Journal of Physical Chemistry A*, **2020**, 124, 1682-1697	2.8
16	Revealing New Atomic-scale Information about Materials by Improving the Quality and Quantifiability of Aberration-corrected STEM Data. *Microscopy and Microanalysis*, **2015**, 21, 2409-2410	0.5
15	Dielectric breakdown along c-axis boundaries in magnetoelectric O2O3 for spintronic devices. *Microscopy and Microanalysis*, **2017**, 23, 1442-1443	0.5
14	Applications of High Precision STEM Imaging to Structurally Complex Materials. *Microscopy and Microanalysis*, **2017**, 23, 418-419	0.5
13	Prospects for Detecting Single Vacancies by Quantitative Scanning Transmission Electron Microscopy. *Microscopy and Microanalysis*, **2015**, 21, 1887-1888	0.5
12	Increased Fluctuation of Interatomic Distances in Distorted Structure of Stoichiometric LaMnO3. *Microscopy and Microanalysis*, **2015**, 21, 2413-2414	0.5
11	Integrated Computational and Experimental Structure Determination for Nanoparticles. *Microscopy and Microanalysis*, **2015**, 21, 2201-2202	0.5
10	Morphology of Amorphous Pockets in SiC Irradiated with 1 MeV Kr Ions. *Microscopy and Microanalysis*, **2014**, 20, 1830-1831	0.5
9	Including Magnetic Contributions in LaMnO3 Defect Models. *ECS Transactions*, **2013**, 50, 91-95	1
8	Head-to-head Inversion Domain Boundaries in Sb-doped p-type ZnO Nanowires. *Microscopy and Microanalysis*, **2012**, 18, 316-317	0.5
7	Approximations for Vibrational Thermodynamics of Disordered Alloys: Effective Supercells and the Quasiharmonic Method. *Materials Research Society Symposia Proceedings*, **1997**, 481, 175	
6	Toward a total energy tight-binding Hamiltonian based on the linear-muffin-tin-orbital method. *Computational Materials Science*, **1997**, 8, 122-130	3.2
5	High-precision stress mapping and defect characterization of thin films of LaMnO 3 grown on DyScO 3 substrate.. *Microscopy and Microanalysis*, **2016**, 22, 1526-1527	0.5
4	Corrigendum to Origin of Fe3+ in Fe-containing, Al-free mantle silicate perovskite[Earth Planet. Sci. Lett. 409 (2014) 319328]. *Earth and Planetary Science Letters*, **2016**, 442, 231-232	5.3
3	Density functional theory modeling of cation diffusion in bulk tetragonal zirconia. *Ceramic Transactions*, **2019**, 95-110	0.1
2	Compositional trends in surface enhanced diffusion in lead silicate glasses. *Computational Materials Science*, **2022**, 206, 111304	3.2

1 CO Oxidation Catalytic Effects of Intrinsic Surface Defects in Rhombohedral LaMnO.. *ChemPhysChem*, **2022**, e202200152 3.2