Dane D Morgan

List of Publications by Year in Descending Order

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	Electronic Structure-Based Descriptors for Oxide Properties and Functions.. *Accounts of Chemical Research*, **2022**,	24.3	5
323	Machine learning in nuclear materials research. *Current Opinion in Solid State and Materials Science*, **2022**, 26, 100975	12	7
322	Molecular dynamic characteristic temperatures for predicting metallic glass forming ability. *Computational Materials Science*, **2022**, 201, 110877	3.2	0
321	Surface Diffusion Is Controlled by Bulk Fragility across All Glass Types.. *Physical Review Letters*, **2022**, 128, 075501	7.4	4
320	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
319	Compositional trends in surface enhanced diffusion in lead silicate glasses. *Computational Materials Science*, **2022**, 206, 111304	3.2	
318	CO Oxidation Catalytic Effects of Intrinsic Surface Defects in Rhombohedral LaMnO.. *ChemPhysChem*, **2022**, e202200152	3.2	
317	Performance and limitations of deep learning semantic segmentation of multiple defects in transmission electron micrographs. *Cell Reports Physical Science*, **2022**, 100876	6.1	1
316	Dopant binding with vacancies and helium in metal hydrides. *Journal of Nuclear Materials*, **2021**, 559, 153437	3.3	0
315	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
314	Graph network based deep learning of bandgaps. *Journal of Chemical Physics*, **2021**, 155, 154702	3.9	3
313	Machine learning principles applied to CT radiomics to predict mucinous pancreatic cysts. *Abdominal Radiology*, **2021**, 1	3	0
312	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
311	Factors correlating to enhanced surface diffusion in metallic glasses. *Journal of Chemical Physics*, **2021**, 154, 104502	3.9	5
310	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
309	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
308	Deciphering water-solid reactions during hydrothermal corrosion of SiC. *Acta Materialia*, **2021**, 209, 116803	8.4	3

307	Mechanisms of bulk and surface diffusion in metallic glasses determined from molecular dynamics simulations. *Acta Materialia*, **2021**, 209, 116794	8.4	7
306	Fast Surface Dynamics on a Metallic Glass Nanowire. *ACS Nano*, **2021**,	16.7	6
305	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
304	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
303	Development and Deployment of Automated Machine Learning Detection in Electron Microcopy Experiments. *Microscopy and Microanalysis*, **2021**, 27, 2136-2137	0.5	2
302	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
301	4D-STEM Determination of Atomic Structure of Amorphous Materials for Renewable Energy Applications. *Microscopy and Microanalysis*, **2021**, 27, 396-398	0.5	0
300	Discovery and engineering of low work function perovskite materials. *Journal of Materials Chemistry C*, **2021**, 9, 12778-12790	7.1	2
299	Exploration of characteristic temperature contributions to metallic glass forming ability. *Computational Materials Science*, **2021**, 196, 110494	3.2	2
298	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
297	An ab-initio based semi-empirical thermal conductivity model for multiphase uranium-zirconium alloys. *Journal of Nuclear Materials*, **2021**, 553, 153044	3.3	1
296	A deep learning based automatic defect analysis framework for In-situ TEM ion irradiations. *Computational Materials Science*, **2021**, 197, 110560	3.2	7
295	Multi defect detection and analysis of electron microscopy images with deep learning. *Computational Materials Science*, **2021**, 199, 110576	3.2	5
294	Molecular simulation-derived features for machine learning predictions of metal glass forming ability. *Computational Materials Science*, **2021**, 199, 110728	3.2	1
293	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	
292	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
291	Opportunities and Challenges for Machine Learning in Materials Science. *Annual Review of Materials Research*, **2020**, 50, 71-103	12.8	60
290	Simulation of Cu precipitation in Fe-Cu dilute alloys with cluster mobility. *Materials and Design*, **2020**, 191, 108574	8.1	8

289	Shape Dependence of Pressure-Induced Phase Transition in CdS Semiconductor Nanocrystals. *Journal of the American Chemical Society*, **2020**, 142, 6505-6510	16.4	20
288	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	
287	Assessing Graph-based Deep Learning Models for Predicting Flash Point. *Molecular Informatics*, **2020**, 39, e1900101	3.8	7
286	Effect of Nonuniform Emission on Miram Curves. *IEEE Transactions on Plasma Science*, **2020**, 48, 146-155	1.3	15
285	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
284	Comment on "Thermal vacancies in random alloys in the single-site mean-field approximation" *Physical Review B*, **2020**, 101,	3.3	4
283	An Unexpected Role of H During SiC Corrosion in Water. *Journal of Physical Chemistry C*, **2020**, 124, 9394-9400	3.8	5
282	Semi-adsorption-controlled growth window for half-Heusler FeVSb epitaxial films. *Physical Review Materials*, **2020**, 4,	3.2	1
281	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
280	Radiation-induced segregation in a ceramic. *Nature Materials*, **2020**, 19, 992-998	27	22
279	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
278	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
277	Understanding the interplay of surface structure and work function in oxides: A case study on SrTiO3. *APL Materials*, **2020**, 8, 071110	5.7	8
276	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
275	Fast approximate STEM image simulations from a machine learning model. *Advanced Structural and Chemical Imaging*, **2019**, 5,	3.9	3
274	Massive Vacancy Concentration Yields Strong Room-Temperature Ferromagnetism in Two-Dimensional ZnO. *Nano Letters*, **2019**, 19, 7085-7092	11.5	18
273	Valleyite: A new magnetic mineral with the sodalite-type structure. *American Mineralogist*, **2019**, 104, 1238-1245	2.9	9
272	Exploring effective charge in electromigration using machine learning. *MRS Communications*, **2019**, 9, 567-575	2.7	8

271	The O-O Bonding and Hydrogen Storage in the Pyrite-type PtO. *Inorganic Chemistry*, **2019**, 58, 8300-8307	5.1	4
270	Tuning perovskite oxides by strain: Electronic structure, properties, and functions in (electro)catalysis and ferroelectricity. *Materials Today*, **2019**, 31, 100-118	21.8	98
269	Factors controlling surface oxygen exchange in oxides. *Nature Communications*, **2019**, 10, 1346	17.4	41
268	Materials Discovery of Stable and Nontoxic Halide Perovskite Materials for High-Efficiency Solar Cells. *Advanced Functional Materials*, **2019**, 29, 1804354	15.6	34
267	New frontiers for the materials genome initiative. *Npj Computational Materials*, **2019**, 5,	10.9	171
266	Error assessment and optimal cross-validation approaches in machine learning applied to impurity diffusion. *Computational Materials Science*, **2019**, 169, 109075	3.2	20
265	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
264	Prediction of concrete coefficient of thermal expansion and other properties using machine learning. *Construction and Building Materials*, **2019**, 220, 587-595	6.7	26
263	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
262	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
261	Density functional theory modeling of cation diffusion in bulk tetragonal zirconia. *Ceramic Transactions*, **2019**, 95-110	0.1	
260	CuMnNiSi precipitate evolution in irradiated reactor pressure vessel steels: Integrated Cluster Dynamics and experiments. *Acta Materialia*, **2019**, 180, 199-217	8.4	15
259	StructOpt: A modular materials structure optimization suite incorporating experimental data and simulated energies. *Computational Materials Science*, **2019**, 160, 1-8	3.2	4
258	Assessing Correlations of Perovskite Catalytic Performance with Electronic Structure Descriptors. *Chemistry of Materials*, **2019**, 31, 785-797	9.6	57
257	Flux effects in precipitation under irradiation: Simulation of Fe-Cr alloys. *Acta Materialia*, **2019**, 164, 586-601	8.4	32
256	Corrosion of Si, C, and SiC in molten salt. *Corrosion Science*, **2019**, 146, 1-9	6.8	14
255	Frontiers in Thermionic Cathode Research. *IEEE Transactions on Electron Devices*, **2018**, 65, 2061-2071	2.9	33
254	A first-principles and experimental study of helium diffusion in periclase MgO. *Physics and Chemistry of Minerals*, **2018**, 45, 641-654	1.6	1

253	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
252	Strain control of oxygen kinetics in the Ruddlesden-Popper oxide LaSrCuO. *Nature Communications*, **2018**, 9, 92	17.4	30
251	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
250	Predicting the thermodynamic stability of perovskite oxides using machine learning models. *Computational Materials Science*, **2018**, 150, 454-463	3.2	95
249	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
248	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
247	Precipitation in Fe-Cu and Fe-Cu-Mn model alloys under irradiation: Dose rate effects. *Acta Materialia*, **2018**, 157, 72-82	8.4	29
246	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
245	Automated defect analysis in electron microscopic images. *Npj Computational Materials*, **2018**, 4,	10.9	54
244	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
243	Transition state redox during dynamical processes in semiconductors and insulators. *NPG Asia Materials*, **2018**, 10, 45-51	10.3	2
242	First-principles investigation on diffusion mechanism of alloying elements in dilute Zr alloys. *Acta Materialia*, **2018**, 154, 161-171	8.4	22
241	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
240	CALPHAD modeling and ab initio calculations of the Np-U-Zr system. *Computational Materials Science*, **2018**, 143, 505-514	3.2	6
239	Factors Controlling Oxygen Interstitial Diffusion in the Ruddlesden□Popper Oxide La2□SrxNiO4+□ *Chemistry of Materials*, **2018**, 30, 7166-7177	9.6	18
238	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
237	Nanoscale Voltage Enhancement at Cathode Interfaces in Li-Ion Batteries. *Chemistry of Materials*, **2017**, 29, 1218-1229	9.6	5
236	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

235	Understanding and reducing deleterious defects in the metastable alloy GaAsBi. *NPG Asia Materials* , **2017**, 9, e345-e345	10.3	19
234	Integrated modeling of second phase precipitation in cold-worked 316 stainless steels under irradiation. *Acta Materialia*, **2017**, 130, 94-110	8.4	23
233	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
232	Atomic Layer Deposited MgO: A Lower Overpotential Coating for Li[NiMnCo]O Cathode. *ACS Applied Materials & Interfaces*, **2017**, 9, 11231-11239	9.5	82
231	Optimization of self-interstitial clusters in 3C-SiC with genetic algorithm. *Journal of Nuclear Materials*, **2017**, 492, 62-73	3.3	8
230	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
229	Continuum model for hydrogen pickup in zirconium alloys of LWR fuel cladding. *Journal of Applied Physics*, **2017**, 121, 135101	2.5	8
228	Robust FCC solute diffusion predictions from ab-initio machine learning methods. *Computational Materials Science*, **2017**, 134, 160-165	3.2	34
227	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
226	Stretching Epitaxial La0.6Sr0.4CoO3 for Fast Oxygen Reduction. *Journal of Physical Chemistry C*, **2017**, 121, 25651-25658	3.8	25
225	Cs diffusion in SiC high-energy grain boundaries. *Journal of Applied Physics*, **2017**, 122, 105901	2.5	2
224	Density-Functional-Theory Modeling of Cation Diffusion in Bulk La1SrxMnO3 (x=0.0 0.25) for Solid-Oxide Fuel-Cell Cathodes. *Physical Review Applied*, **2017**, 8,	4.3	8
223	Strain effects on oxygen vacancy formation energy in perovskites. *Solid State Ionics*, **2017**, 311, 105-117	3.3	21
222	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
221	Increased stability of CuZrAl metallic glasses prepared by physical vapor deposition. *Journal of Alloys and Compounds*, **2017**, 728, 1110-1115	5.7	15
220	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
219	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
218	Local Dielectric Breakdown Path along c-Axis Planar Boundaries in Cr2O3 Thin Films. *Advanced Materials Interfaces*, **2017**, 4, 1700172	4.6	11

217	Work function and surface stability of tungsten-based thermionic electron emission cathodes. *APL Materials*, **2017**, 5, 116105	5.7	35
216	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
215	The MAterials Simulation Toolkit (MAST) for atomistic modeling of defects and diffusion. *Computational Materials Science*, **2017**, 126, 90-102	3.2	24
214	High-throughput computational screening for low work function perovskite electron emitters **2017** ,		1
213	Dielectric breakdown along c-axis boundaries in magnetoelectric O2O3 for spintronic devices. *Microscopy and Microanalysis*, **2017**, 23, 1442-1443	0.5	
212	Bayesian Statistical Model for Imaging of Single La Vacancies in LaMnO3. *Microscopy and Microanalysis*, **2017**, 23, 1572-1573	0.5	2
211	Applications of High Precision STEM Imaging to Structurally Complex Materials. *Microscopy and Microanalysis*, **2017**, 23, 418-419	0.5	
210	Polarity-driven oxygen vacancy formation in ultrathin LaNiO3 films on SrTiO3. *Physical Review Materials*, **2017**, 1,	3.2	19
209	Ab initio prediction of threshold displacement energies in ZrC. *Journal of Nuclear Materials*, **2016**, 471, 214-219	3.3	11
208	Exposing New Atomic-scale Information about Materials by Improving the Quality and Quantifiability of Aberration-corrected STEM Data **2016**, 495-496		
207	Nanoparticle Structure from Genetic Algorithm Refinement Against Quantitative STEM Data **2016**, 521-522		
206	Factors controlling oxygen migration barriers in perovskites. *Solid State Ionics*, **2016**, 296, 71-77	3.3	48
205	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
204	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
203	Ab initio energetics for modeling phase stability of the Np-U system. *Journal of Nuclear Materials*, **2016**, 479, 260-270	3.3	2
202	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
201	High-throughput ab-initio dilute solute diffusion database. *Scientific Data*, **2016**, 3, 160054	8.2	71
200	Nanometre-thick single-crystalline nanosheets grown at the water-air interface. *Nature Communications*, **2016**, 7, 10444	17.4	100

199	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
198	Microstructural Evolution of Type 304 and 316 Stainless Steels Under Neutron Irradiation at LWR Relevant Conditions. *Jom*, **2016**, 68, 517-529	2.1	20
197	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
196	Effect of carbon ion irradiation on Ag diffusion in SiC. *Journal of Nuclear Materials*, **2016**, 471, 220-232	3.3	9
195	Three-Dimensional Imaging of Single La Vacancies in LaMnO 3. *Microscopy and Microanalysis*, **2016**, 22, 902-903	0.5	2
194	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
193	Understanding and Controlling the Work Function of Perovskite Oxides Using Density Functional Theory. *Advanced Functional Materials*, **2016**, 26, 5471-5482	15.6	75
192	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
191	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
190	High-throughput computational design of cathode coatings for Li-ion batteries. *Nature Communications*, **2016**, 7, 13779	17.4	112
189	Thermal diffusion boron doping of single-crystal natural diamond. *Journal of Applied Physics*, **2016**, 119, 205703	2.5	22
188	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	
187	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
186	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
185	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	
184	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
183	Integrated Computational and Experimental Structure Refinement for Nanoparticles. *ACS Nano*, **2016**, 10, 4031-8	16.7	20
182	Response to letter Electron correlation and relativity of the 5f electrons in the U Zr alloy system *Journal of Nuclear Materials*, **2016**, 476, 110-112	3.3	3

181	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
180	Oxygen Point Defect Chemistry in Ruddlesden-Popper Oxides (La1-xSrx)2MO4□□(M = Co, Ni, Cu). *Journal of Physical Chemistry Letters*, **2016**, 7, 1939-44	6.4	37
179	Radiation-induced mobility of small defect clusters in covalent materials. *Physical Review B*, **2016**, 94,	3.3	8
178	Defect kinetics and resistance to amorphization in zirconium carbide. *Journal of Nuclear Materials*, **2015**, 457, 343-351	3.3	18
177	Lithium transport through lithium-ion battery cathode coatings. *Journal of Materials Chemistry A*, **2015**, 3, 17248-17272	13	82
176	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
175	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
174	Thermodynamic and kinetic modeling of oxide precipitation in nanostructured ferritic alloys. *Acta Materialia*, **2015**, 91, 340-354	8.4	35
173	Grain boundary character dependence of radiation-induced segregation in a model Ni□r alloy. *Journal of Materials Research*, **2015**, 30, 1290-1299	2.5	29
172	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
171	Grain boundary diffusion of Ag through polycrystalline SiC in TRISO fuel particles. *Journal of Nuclear Materials*, **2015**, 467, 332-340	3.3	12
170	Genetic algorithm optimization of defect clusters in crystalline materials. *Computational Materials Science*, **2015**, 98, 234-244	3.2	25
169	Strain effects on oxygen migration in perovskites. *Physical Chemistry Chemical Physics*, **2015**, 17, 2715-21	3.6	61
168	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
167	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	
166	First-principles studies on molecular beam epitaxy growth of GaAs1□Bix. *Physical Review B*, **2015**, 92,	3.3	10
165	Strain-compensated GaAs1□Py/GaAs1□Biz/GaAs1□Pyquantum wells for laser applications. *Semiconductor Science and Technology*, **2015**, 30, 094011	1.8	6
164	Prospects for Detecting Single Vacancies by Quantitative Scanning Transmission Electron Microscopy. *Microscopy and Microanalysis*, **2015**, 21, 1887-1888	0.5	

163	Increased Fluctuation of Interatomic Distances in Distorted Structure of Stoichiometric LaMnO3. *Microscopy and Microanalysis*, **2015**, 21, 2413-2414	0.5	
162	Integrated Computational and Experimental Structure Determination for Nanoparticles. *Microscopy and Microanalysis*, **2015**, 21, 2201-2202	0.5	
161	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
160	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
159	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
158	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
157	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
156	Local strain effect on the band gap engineering of graphene by a first-principles study. *Applied Physics Letters*, **2015**, 106, 053113	3.4	23
155	Origin of Fe3+ in Fe-containing, Al-free mantle silicate perovskite. *Earth and Planetary Science Letters*, **2015**, 409, 319-328	5.3	14
154	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
153	Massive interfacial reconstruction at misfit dislocations in metal/oxide interfaces. *Scientific Reports*, **2014**, 4, 6533	4.9	27
152	Effect of Grain Boundary Stresses on Sink Strength. *Materials Research Letters*, **2014**, 2, 100-106	7.4	40
151	Joint experimental and computational 17O solid state NMR study of Brownmillerite Ba2In2O5. *Physical Chemistry Chemical Physics*, **2014**, 16, 2597-606	3.6	7
150	Structures and stabilities of small carbon interstitial clusters in cubic silicon carbide. *Acta Materialia*, **2014**, 62, 162-172	8.4	17
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