Mark Asta

List of Publications by Citations

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143	10,560	46	102
papers	citations	h-index	g-index
147	12,909	7.4	6.43
ext. papers	ext. citations	avg, IF	L-index

#	Paper	IF	Citations
143	Development of new interatomic potentials appropriate for crystalline and liquid iron. *Philosophical Magazine*, **2003**, 83, 3977-3994	1.6	941
142	The alloy theoretic automated toolkit: A user guide. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2002**, 26, 539-553	1.9	868
141	Efficient stochastic generation of special quasirandom structures. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2013**, 42, 13-18	1.9	572
140	Lead-free germanium iodide perovskite materials for photovoltaic applications. *Journal of Materials Chemistry A*, **2015**, 3, 23829-23832	13	569
139	Charting the complete elastic properties of inorganic crystalline compounds. *Scientific Data*, **2015**, 2, 150009	8.2	428
138	Method for computing the anisotropy of the solid-liquid interfacial free energy. *Physical Review Letters*, **2001**, 86, 5530-3	7.4	389
137	Atomistic modeling of interfaces and their impact on microstructure and properties. *Acta Materialia*, **2010**, 58, 1117-1151	8.4	379
136	First-principles theory of ionic diffusion with nondilute carriers. *Physical Review B*, **2001**, 64,	3.3	337
135	Analysis of semi-empirical interatomic potentials appropriate for simulation of crystalline and liquid Al and Cu. *Philosophical Magazine*, **2008**, 88, 1723-1750	1.6	284
134	Crystal-melt interfacial free energies in hcp metals: A molecular dynamics study of Mg. *Physical Review B*, **2006**, 73,	3.3	281
133	Short-range order and its impact on the CrCoNi medium-entropy alloy. *Nature*, **2020**, 581, 283-287	50.4	254
132	Tunable stacking fault energies by tailoring local chemical order in CrCoNi medium-entropy alloys. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 8919-8924	11.5	251
131	Structural phase transformations in metallic grain boundaries. *Nature Communications*, **2013**, 4, 1899	17.4	238
130	Matminer: An open source toolkit for materials data mining. *Computational Materials Science*, **2018**, 152, 60-69	3.2	221
129	Metallurgy. Origin of dramatic oxygen solute strengthening effect in titanium. *Science*, **2015**, 347, 635-9	33.3	189
128	Solution-Processed Tin-Based Perovskite for Near-Infrared Lasing. *Advanced Materials*, **2016**, 28, 8191-8196	24	174
127	High-throughput computational screening of thermal conductivity, Debye temperature, and Grüneisen parameter using a quasiharmonic Debye model. *Physical Review B*, **2014**, 90,	3.3	172

126	Dipolar cations confer defect tolerance in wide-bandgap metal halide perovskites. *Nature Communications*, **2018**, 9, 3100	17.4	171
125	Test of the universal scaling law for the diffusion coefficient in liquid metals. *Physical Review Letters*, **2000**, 85, 594-7	7.4	156
124	Atomistic computation of liquid diffusivity, solid-liquid interfacial free energy, and kinetic coefficient in Au and Ag. *Physical Review B*, **2002**, 65,	3.3	148
123	Morphology-Independent Stable White-Light Emission from Self-Assembled Two-Dimensional Perovskites Driven by Strong Exciton□Phonon Coupling to the Organic Framework. *Chemistry of Materials*, **2017**, 29, 3947-3953	9.6	146
122	Rational Design: A High-Throughput Computational Screening and Experimental Validation Methodology for Lead-Free and Emergent Hybrid Perovskites. *ACS Energy Letters*, **2017**, 2, 837-845	20.1	142
121	A Statistical Learning Framework for Materials Science: Application to Elastic Moduli of k-nary Inorganic Polycrystalline Compounds. *Scientific Reports*, **2016**, 6, 34256	4.9	142
120	Understanding thermoelectric properties from high-throughput calculations: trends, insights, and comparisons with experiment. *Journal of Materials Chemistry C*, **2016**, 4, 4414-4426	7.1	139
119	Computational Study of Halide Perovskite-Derived A2BX6 Inorganic Compounds: Chemical Trends in Electronic Structure and Structural Stability. *Chemistry of Materials*, **2017**, 29, 7740-7749	9.6	128
118	Calculation of alloy solid-liquid interfacial free energies from atomic-scale simulations. *Physical Review B*, **2002**, 66,	3.3	118
117	A database to enable discovery and design of piezoelectric materials. *Scientific Data*, **2015**, 2, 150053	8.2	114
116	Evaluation of the constant potential method in simulating electric double-layer capacitors. *Journal of Chemical Physics*, **2014**, 141, 184102	3.9	105
115	Phase stability, phase transformations, and elastic properties of Cu6Sn5: Ab initio calculations and experimental results. *Journal of Materials Research*, **2005**, 20, 3102-3117	2.5	105
114	Segregation-induced phase transformations in grain boundaries. *Physical Review B*, **2015**, 92,	3.3	100
113	Development of interatomic potentials appropriate for simulation of solid□liquid interface properties in Al□Mg alloys. *Philosophical Magazine*, **2009**, 89, 3269-3285	1.6	97
112	First-principles study of phase stability of Ti□Al intermetallic compounds. *Journal of Materials Research*, **1993**, 8, 2554-2568	2.5	88
111	Probing the Stability and Band Gaps of Cs2AgInCl6 and Cs2AgSbCl6 Lead-Free Double Perovskite Nanocrystals. *Chemistry of Materials*, **2019**, 31, 3134-3143	9.6	84
110	Universal structural parameter to quantitatively predict metallic glass properties. *Nature Communications*, **2016**, 7, 13733	17.4	84
109	Crystal-melt interfacial free energies in metals: fcc versus bcc. *Physical Review B*, **2004**, 69,	3.3	83

108	A first-principles approach to modeling alloy phase equilibria. *Jom*, **2001**, 53, 16-19	2.1	66
107	Computational and Experimental Investigation of Ti Substitution in Li1(NixMnxCo1-2x-yTiy)O2 for Lithium Ion Batteries. *Journal of Physical Chemistry Letters*, **2014**, 5, 3649-55	6.4	64
106	Atomistic Simulation Methods for Computing the Kinetic Coefficient in Solid-Liquid Systems. *Journal of Materials Science*, **2002**, 10, 181-189		64
105	Density of constitutional and thermal point defects in L12 Al3Sc. *Physical Review B*, **2001**, 63,	3.3	54
104	Predicting defect behavior in B2 intermetallics by merging ab initio modeling and machine learning. *Npj Computational Materials*, **2016**, 2,	10.9	54
103	Three-State Ferroelastic Switching and Large Electromechanical Responses in PbTiO Thin Films. *Advanced Materials*, **2017**, 29, 1702069	24	53
102	Theoretical prediction of high melting temperature for a MoRuTaW HCP multiprincipal element alloy. *Npj Computational Materials*, **2021**, 7,	10.9	51
101	Electron transport and visible light absorption in a plasmonic photocatalyst based on strontium niobate. *Nature Communications*, **2017**, 8, 15070	17.4	48
100	Second-Nearest-Neighbor Correlations from Connection of Atomic Packing Motifs in Metallic Glasses and Liquids. *Scientific Reports*, **2015**, 5, 17429	4.9	47
99	An efficient and accurate framework for calculating lattice thermal conductivity of solids: AFLOW-AAPL Automatic Anharmonic Phonon Library. *Npj Computational Materials*, **2017**, 3,	10.9	46
98	Spatial correlation of elastic heterogeneity tunes the deformation behavior of metallic glasses. *Npj Computational Materials*, **2018**, 4,	10.9	46
97	High-throughput Computational Study of Halide Double Perovskite Inorganic Compounds. *Chemistry of Materials*, **2019**, 31, 5392-5401	9.6	46
96	A hierarchical microstructure due to chemical ordering in the bcc lattice: Early stages of formation in a ferritic FeAlCrNiTi alloy. *Acta Materialia*, **2015**, 92, 220-232	8.4	45
95	YCuTe2: a member of a new class of thermoelectric materials with CuTe4-based layered structure. *Journal of Materials Chemistry A*, **2016**, 4, 2461-2472	13	43
94	Density functional theory based calculation of small-polaron mobility in hematite. *Physical Review B* , **2014**, 89,	3.3	43
93	Structural and vibrational properties of MoO3 from van der Waals corrected density functional theory calculations. *Physical Review B*, **2012**, 85,	3.3	42
92	Molecular dynamics simulations of the crystal-melt interfacial free energy and mobility in Mo and V. *Philosophical Magazine*, **2006**, 86, 3651-3664	1.6	40
91	Combining the AFLOW GIBBS and elastic libraries to efficiently and robustly screen thermomechanical properties of solids. *Physical Review Materials*, **2017**, 1,	3.2	38

90	First-principles investigation of perfect and diffuse antiphase boundaries in HCP-based Ti-Al alloys. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2002**, 33, 735-741	2.3	35
89	Anomalous structure-property relationships in metallic glasses through pressure-mediated glass formation. *Physical Review B*, **2016**, 93,	3.3	33
88	On the formation of hierarchically structured L2 1 -Ni2TiAl type precipitates in a ferritic alloy. *Journal of Materials Science*, **2013**, 48, 2067-2075	4.3	33
87	Direct imaging of short-range order and its impact on deformation in Ti-6Al. *Science Advances*, **2019** , 5, eaax2799	14.3	32
86	Defect reconfiguration in a Ti-Al alloy via electroplasticity. *Nature Materials*, **2021**, 20, 468-472	27	32
85	Tunable and low-loss correlated plasmons in Mott-like insulating oxides. *Nature Communications*, **2017**, 8, 15271	17.4	30
84	Direct measurement of nanostructural change during in situ deformation of a bulk metallic glass. *Nature Communications*, **2019**, 10, 2445	17.4	30
83	Ab initio modeling of the energy landscape for screw dislocations in body-centered cubic high-entropy alloys. *Npj Computational Materials*, **2020**, 6,	10.9	30
82	Ab initio simulations of molten Ni alloys. *Journal of Applied Physics*, **2010**, 107, 113522	2.5	29
81	Actinide Dioxides in Water: Interactions at the Interface. *Journal of Physical Chemistry Letters*, **2011**, 2, 3130-3134	6.4	29
80	Vacancy-Ordered Double Perovskite CsTeI Thin Films for Optoelectronics. *Chemistry of Materials*, **2020**, 32, 6676-6684	9.6	26
79	Determining the range of forces in empirical many-body potentials using first-principles calculations. *Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties*, **2001**, 81, 991-1008		25
78	The chain of chirality transfer in tellurium nanocrystals. *Science*, **2021**, 372, 729-733	33.3	24
77	Electronic Origins of Anomalous Twin Boundary Energies in Hexagonal Close Packed Transition Metals. *Physical Review Letters*, **2015**, 115, 065501	7.4	22
76	Ideal strength and ductility in metals from second- and third-order elastic constants. *Physical Review B*, **2017**, 96,	3.3	22
75	van der Waals density functional study of CO2 binding in zeolitic imidazolate frameworks. *Physical Review B*, **2012**, 85,	3.3	22
74	Energetics of {105}-faceted Ge nanowires on Si(001): An atomistic calculation of edge contributions. *Physical Review B*, **2007**, 75,	3.3	22
73	Ab initio molecular-dynamics study of highly nonideal structural and thermodynamic properties of liquid Ni-Al alloys. *Physical Review B*, **2001**, 64,	3.3	22

72	First-principles study of the structural and elastic properties of rhenium-based transition-metal alloys. *Physical Review B*, **2012**, 86,	3.3	21
71	Atomistic simulations of dislocation mobility in refractory high-entropy alloys and the effect of chemical short-range order. *Nature Communications*, **2021**, 12, 4873	17.4	21
70	On the question of fractal packing structure in metallic glasses. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 8458-8463	11.5	20
69	Chemical ordering in substituted fluorite oxides: a computational investigation of HoZrO and REThO (RE=Ho, Y, Gd, Nd, La). *Scientific Reports*, **2016**, 6, 38772	4.9	19
68	Melts of CrCoNi-based high-entropy alloys: Atomic diffusion and electronic/atomic structure from ab initio simulation. *Applied Physics Letters*, **2018**, 113, 111902	3.4	17
67	PyDII: A python framework for computing equilibrium intrinsic point defect concentrations and extrinsic solute site preferences in intermetallic compounds. *Computer Physics Communications*, **2015**, 193, 118-123	4.2	16
66	Orientation-dependent properties of epitaxially strained perovskite oxide thin films: Insights from first-principles calculations. *Physical Review B*, **2017**, 95,	3.3	16
65	Temperature dependence of the structure and shear response of a Σ11 asymmetric tilt grain boundary in copper from molecular-dynamics. *Philosophical Magazine*, **2012**, 92, 4320-4333	1.6	16
64	High-throughput calculations in the context of alloy design. *MRS Bulletin*, **2019**, 44, 252-256	3.2	15
63	Frontiers in strain-engineered multifunctional ferroic materials. *MRS Communications*, **2016**, 6, 151-166	2.7	15
62	Experimental and Computational Investigation of Lepidocrocite Anodes for Sodium-Ion Batteries. *Chemistry of Materials*, **2016**, 28, 4284-4291	9.6	15
61	Targeted Synthesis of Trimeric Organic Bromoplumbate Hybrids That Display Intrinsic, Highly Stokes-Shifted, Broadband Emission. *Chemistry of Materials*, **2020**, 32, 4431-4441	9.6	14
60	Step free energies at faceted solid surfaces: Theory and atomistic calculations for steps on the Cu(111) surface. *Physical Review B*, **2017**, 95,	3.3	14
59	Capillary force induced structural deformation in liquid infiltrated elastic circular tubes. *Physical Review B*, **2010**, 81,	3.3	14
58	Bubble nucleation and migration in a lead-iron hydr(oxide) core-shell nanoparticle. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 12928-32	11.5	13
57	First-principles theory of nanoscale pattern formation in ultrathin alloy films: A comparative study of Fe-Ag on Ru(0001) and Mo(110) substrates. *Physical Review B*, **2008**, 77,	3.3	13
56	Mechanistic basis of oxygen sensitivity in titanium. *Science Advances*, **2020**, 6,	14.3	13
55	Magnetically driven short-range order can explain anomalous measurements in CrCoNi. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	13

54	Structure of liquid Al and Al67Mg33 alloy: comparison between experiment and simulation. *Philosophical Magazine*, **2014**, 94, 1876-1892	1.6	12
53	Bistable Amphoteric Native Defect Model of Perovskite Photovoltaics. *Journal of Physical Chemistry Letters*, **2018**, 9, 3878-3885	6.4	11
52	First-principles investigation of perfect and diffuse antiphase boundaries in HCP-based Ti-Al alloys **2002**, 33, 735		10
51	NMR Crystallography: Evaluation of Hydrogen Positions in Hydromagnesite by C{ H} REDOR Solid-State NMR and Density Functional Theory Calculation of Chemical Shielding Tensors. *Angewandte Chemie - International Edition*, **2019**, 58, 4210-4216	16.4	9
50	Free energy of grain boundary phases: Atomistic calculations for Σ5(310)[001] grain boundary in Cu. *Physical Review Materials*, **2018**, 2,	3.2	9
49	Giant isotope effect on phonon dispersion and thermal conductivity in methylammonium lead iodide. *Science Advances*, **2020**, 6, eaaz1842	14.3	9
48	Calculations of planar defect energies in substitutional alloys using the special-quasirandom-structure approach. *Physical Review B*, **2016**, 93,	3.3	8
47	Convergence of calculated dislocation core structures in hexagonal close packed titanium. *Modelling and Simulation in Materials Science and Engineering*, **2018**, 26, 014003	2	8
46	Identifying rhenium substitute candidate multiprincipal-element alloys from electronic structure and thermodynamic criteria. *Journal of Materials Research*, **2019**, 34, 3296-3304	2.5	7
45	Effect of non-Schmid stresses on <a>-type screw dislocation core structure and mobility in titanium. *Computational Materials Science*, **2019**, 161, 261-264	3.2	7
44	First principles study of pyrophosphate defects and dopant–defect interactions in stronium-doped lanthanum orthophosphate. *Journal of Materials Chemistry A*, **2014**, 2, 1047-1053	13	6
43	Universal nature of the saddle states of structural excitations in metallic glasses. *Materials Today Physics*, **2021**, 17, 100359	8	6
42	Insights into dislocation climb efficiency in FCC metals from atomistic simulations. *Acta Materialia*, **2020**, 193, 172-181	8.4	5
41	Computational Materials Discovery and Design. *Jom*, **2014**, 66, 364-365	2.1	5
40	First-principles studies of proton-Ba interactions in doped LaPO4. *Journal of Materials Chemistry*, **2012**, 22, 3758		5
39	Lattice Dynamics and Optoelectronic Properties of Vacancy-Ordered Double Perovskite Cs2TeX6 (X = Cl□Br□I)Single Crystals. *Journal of Physical Chemistry C*, **2021**, 125, 25126-25139	3.8	5
38	Dislocation content of grain boundary phase junctions and its relation to grain boundary excess properties. *Physical Review B*, **2021**, 103,	3.3	5
37	Twin nucleation from a single dislocation in hexagonal close-packed crystals. *Acta Materialia*, **2021**, 202, 35-41	8.4	5

36	Quantum effects on dislocation motion from ring-polymer molecular dynamics. *Npj Computational Materials*, **2018**, 4,	10.9	5
35	Epitaxial phase diagrams of SrTiO3, CaTiO3, and SrHfO3: Computational investigation including the role of antiferrodistortive and A-site displacement modes. *Physical Review B*, **2018**, 97,	3.3	4
34	Electronic and Polar Properties of Vanadate Compounds Stabilized by Epitaxial Strain. *Chemistry of Materials*, **2018**, 30, 5870-5877	9.6	4
33	Soft-phonon feature, site defects, and a frustrated phase transition in Ni50Ti47Fe3: Experiments and first-principles calculations. *Physical Review B*, **2008**, 77,	3.3	4
32	Computing elastic anisotropy to discover gum-metal-like structural alloys. *Physical Review Materials* , **2017**, 1,	3.2	4
31	Elimination of oxygen sensitivity in □itanium by substitutional alloying with Al. *Nature Communications*, **2021**, 12, 6158	17.4	4
30	Transmission Electron Microscopy (TEM) Study of the Oxide Layers Formed on Fe-12Cr-4Al Ferritic Alloy in an Oxygenated Pb-Bi Environment at 800□C. *Jom*, **2018**, 70, 1471-1477	2.1	3
29	Stability of strained thin films with interface misfit dislocations: A multiscale computational study. *Thin Solid Films*, **2010**, 519, 809-817	2.2	3
28	A First-Principles Study of the Phase Stability of FCC-and HCP-Based Ti-Al Alloys. *Materials Research Society Symposia Proceedings*, **1992**, 288, 153		3
27	Kinetics of Crystallization and Orientational Ordering in Dipolar Particle Systems. *Crystal Growth and Design*, **2020**, 20, 7862-7873	3.5	3
26	Ab-initio simulation studies of chromium solvation in molten fluoride salts. *Journal of Molecular Liquids*, **2021**, 335, 116351	6	3
25	First-principles thermal compatibility between Ru-based Re-substitute alloys and Ir coatings. *Computational Materials Science*, **2019**, 170, 109199	3.2	2
24	Phase transformation pathways of ultrafast-laser-irradiated Ln2O3(Ln=Er□u). *Physical Review B*, **2018**, 97,	3.3	2
23	Multiscale modeling of submonolayer growth for Fe/Mo (110). *European Physical Journal B*, **2013**, 86, 1	1.2	2
22	NMR Crystallography: Evaluation of Hydrogen Positions in Hydromagnesite by 13C{1H} REDOR Solid-State NMR and Density Functional Theory Calculation of Chemical Shielding Tensors. *Angewandte Chemie*, **2019**, 131, 4254-4260	3.6	1
21	Examination of the electronic structure of crystalline and liquid Al versus temperature by in situ electron energy-loss spectroscopy (EELS). *Micron*, **2015**, 76, 14-8	2.3	1
20	Computational Materials Science and Engineering Education: An Updated Survey of Trends and Needs. *Jom*, **2018**, 70, 1644-1651	2.1	1
19	Capillary fluctuations of surface steps: An atomistic simulation study for the model Cu(111) system. *Physical Review E*, **2017**, 96, 043308	2.4	1

18	JOM-e: The symposium on computational methods in materials education. *Jom*, **2003**, 55, 13-13	2.1	1
17	Phase Transformations in Hexagonal-Close-Packed Alloys: Analysis with the Cluster Variation Method. *Materials Research Society Symposia Proceedings*, **1992**, 291, 395		1
16	Thermodynamic model for polymorphic dislocation core spreading within hexagonal close packed metals. *Physical Review Materials*, **2022**, 6,	3.2	1
15	Modeling the effect of short-range order on cross-slip in an FCC solid solution. *Acta Materialia*, **2022**, 226, 117615	8.4	1
14	Molecular dynamics studies of <a> -type screw dislocation core structure polymorphism in titanium. *Physical Review Materials*, **2022**, 6,	3.2	1
13	Evaluating the effects of pillar shape and gallium ion beam damage on the mechanical properties of single crystal aluminum nanopillars. *Journal of Materials Research*, **2021**, 36, 2515-2528	2.5	1
12	Origin and Quenching of Novel ultraviolet and blue emission in NdGaO3: Concept of Super-Hydrogenic Dopants. *Scientific Reports*, **2016**, 6, 36352	4.9	1
11	The effect of Cr alloying on defect migration at Ni grain boundaries. *Journal of Materials Science*,1	4.3	0
10	Screw dislocation mobility in a face-centered cubic solid solution with short-range order. *Scripta Materialia*, **2022**, 210, 114465	5.6	0
9	In situ observations and measurements of plastic deformation, phase transformations and fracture with 4D-STEM. *Microscopy and Microanalysis*, **2021**, 27, 1494-1495	0.5	0
8	Anomalous size effect on yield strength enabled by compositional heterogeneity in high-entropy alloy nanoparticles.. *Nature Communications*, **2022**, 13, 2789	17.4	0
7	Understanding the Slip Planarity and Residual Strain Field in Ti-6Al using Nanobeam Electron Diffraction and First Principles Calculations. *Microscopy and Microanalysis*, **2019**, 25, 1892-1893	0.5	
6	Summary report of CALPHAD XLI Berkeley, California, USA, 2012. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2014**, 45, 204-250	1.9	
5	Molecular-Dynamics Simulations of Molten Ni-Based Superalloys **2012**, 537-545		
4	Hierarchically Structured Precipitates in a Ferritic Alloy Characterized by Diffraction Contrast and Energy Filtered Imaging. *Microscopy and Microanalysis*, **2012**, 18, 1472-1473	0.5	
3	First-principles calculation of the effect of strain on the diffusion of Ge adatoms on Si and Ge (001) surfaces. *Materials Research Society Symposia Proceedings*, **2002**, 749, 1		
2	A First-Principles Study of the Phase Stability of FCC-Based Ti-Al Alloys. *Materials Research Society Symposia Proceedings*, **1992**, 278, 313		
1	Molecular-Dynamics Simulations of NI-Based Superalloys325-329		