Raymundo Arroyave

List of Publications by Year
in descending order

203	6,284	61857	98622
papers	citations	43 h-index	67 g-index

209	209	209	5059
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ab initio lattice stability in comparison with CALPHAD lattice stability. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2004, 28, 79-90.	0.7	340
2	First-Principles Calculation of Self-Diffusion Coefficients. Physical Review Letters, 2008, 100, 215901.	2.9	231
3	TEM study of structural and microstructural characteristics of a precipitate phase in Ni-rich Niâ€“Tiâ€“Hf and Niâ€“Tiâ€“Zr shape memory alloys. Acta Materialia, 2013, 61, 6191-6206.	3.8	169
4	An ultra-high strength martensitic steel fabricated using selective laser melting additive manufacturing: Densification, microstructure, and mechanical properties. Acta Materialia, 2020, 186, 199-214.	3.8	151
5	Assessing printability maps in additive manufacturing of metal alloys. Acta Materialia, 2019, 176, 199-210.	3.8	146
6	Thermodynamic properties of binary hcp solution phases from special quasirandom structures. Physical Review B, 2006, 74, .	1.1	122
7	Spatial Control of Functional Response in 4D-Printed Active Metallic Structures. Scientific Reports, 2017, 7, 46707.	1.6	109
8	Thermodynamic assessment of the Cuâ€“Tiâ€“Zr system. Journal of Alloys and Compounds, 2003, 351, 158-170.	2.8	102
9	Thermodynamic modeling of the Hfâ€“Siâ€“O system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2006, 30, 375-386.	0.7	98
10	Ab initio thermodynamic properties of stoichiometric phases in the Niâ€“Al system. Acta Materialia, 2005, 53, 1809-1819.	3.8	96
11	Phase-field simulations of intermetallic compound growth in Cu/Sn/Cu sandwich structure under transient liquid phase bonding conditions. Acta Materialia, 2012, 60, 6278-6287.	3.8	95
12	Tailored thermal expansion alloys. Acta Materialia, 2016, 102, 333-341.	3.8	92
13	Early stages of intermetallic compound formation and growth during lead-free soldering. Acta Materialia, 2010, 58, 4900-4910.	3.8	88
14	Complex magnetic ordering as a driving mechanism of multifunctional properties of Heusler alloys from first principles. European Physical Journal B, 2013, 86, 1.	0.6	88
15	Phase equilibria, thermodynamics and solidification microstructures of Mgâ€“Snâ€“Ca alloys, Part 1: Experimental investigation and thermodynamic modeling of the ternary Mgâ€“Snâ€“Ca system. Intermetallics, 2008, 16, 299-315.	1.8	86
16	Multi-objective Bayesian materials discovery: Application on the discovery of precipitation strengthened NiTi shape memory alloys through micromechanical modeling. Materials and Design, 2018, 160, 810-827.	3.3	83
17	Finite interface dissipation phase field modeling of Niâ€“Nb under additive manufacturing conditions. Acta Materialia, 2020, 185, 320-339.	3.8	83
18	Laser Powder Bed Fusion of Defect-Free NiTi Shape Memory Alloy Parts with Superior Tensile Superelasticity. Acta Materialia, 2022, 229, 117781.	3.8	79

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19	Controlling martensitic transformation characteristics in defect-free NiTi shape memory alloys fabricated using laser powder bed fusion and a process optimization framework. Acta Materialia, 2021, 215, 117017.	3.8	78
20	Mapping mechanisms and growth regimes of magnesium electrodeposition at high current densities. Materials Horizons, 2020, 7, 843-854.	6.4	77
21	Concurrent nucleation, formation and growth of two intermetallic compounds (Cu6Sn5 and Cu3Sn) during the early stages of lead-free soldering. Acta Materialia, 2012, 60, 923-934.	3.8	75
22	On the printability and transformation behavior of nickel-titanium shape memory alloys fabricated using laser powder-bed fusion additive manufacturing. Journal of Manufacturing Processes, 2018, 35, 672-680.	2.8	75
23	First-principles calculation of the instability leading to giant inverse magnetocaloric effects. Physical Review B, 2014, 89, .	1.1	73
24	Multi-phase microstructure design of a low-alloy TRIP-assisted steel through a combined computational and experimental methodology. Acta Materialia, 2012, 60, 3022-3033.	3.8	71
25	On the microstructural origins of martensitic transformation arrest in a NiCoMnIn magnetic shape memory alloy. Acta Materialia, 2018, 142, 95-106.	3.8	67
26	Thermodynamic modeling of the Zrî—¸O system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2002, 26, 95-118.	0.7	65
27	First-principles calculations of the Znâ€“Zr system. Acta Materialia, 2006, 54, 473-482.	3.8	65
28	Phase stability inÎ±- andÎ²-rhombohedral boron. Physical Review B, 2007, 75, .	1.1	64
29	Efficient exploration of the High Entropy Alloy composition-phase space. Acta Materialia, 2018, 152, 41-57.	3.8	62
30	Numerical and experimental analysis of heat distribution in the laser powder bed fusion of Ti-6Al-4V. IISE Transactions, 2019, 51, 136-152.	1.6	62
31	Structural, physical and mechanical properties of Ti3(Al1â^'xSix)C2 solid solution with x=0â€“1. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2016, 676, 197-208.	2.6	60
32	Accelerated design of Fe-based soft magnetic materials using machine learning and stochastic optimization. Acta Materialia, 2020, 194, 144-155.	3.8	60
33	Real-time atomistic observation of structural phase transformations in individual hafnia nanorods. Nature Communications, 2017, 8, 15316.	5.8	59
34	Autonomous efficient experiment design for materials discovery with Bayesian model averaging. Physical Review Materials, 2018, 2, .	0.9	58
35	Thermodynamic modelling of the Znâ€“Zr system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2006, 30, 1-13.	0.7	57
36	A Sensory Material Approach for Reducing Variability in Additively Manufactured Metal Parts. Scientific Reports, 2017, 7, 3604.	1.6	55

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37	A Firstâ€Principles Investigation of the Compositional Dependent Properties of Magnetic Shape Memory Heusler Alloys. Advanced Engineering Materials, 2012, 14, 530-546.	1.6	54
38	Early stage growth characteristics of Ag 3 Sn intermetallic compounds during solidâ€“solid and solidâ€“liquid reactions in the Agâ€“Sn interlayer system: Experiments and simulations. Journal of Alloys and Compounds, 2014, 617, 763-773.	2.8	53
39	Metal substrate effects on the thermochemistry of active brazing interfaces. Acta Materialia, 2003, 51, 4871-4880.	3.8	52
40	Systems Approaches to Materials Design: Past, Present, and Future. Annual Review of Materials Research, 2019, 49, 103-126.	4.3	49
41	Revisiting thermodynamics and kinetic diffusivities of uraniumâ€“niobium with Bayesian uncertainty analysis. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2016, 55, 219-230.	0.7	46
42	Intermetallics in theMgâ˜'Caâ˜'Snternary system: Structural, vibrational, and thermodynamic properties from first principles. Physical Review B, 2006, 74, .	1.1	45
43	Multiple ferroic glasses via ordering. Acta Materialia, 2015, 101, 107-115.	3.8	45
44	Phase-field simulations of intermetallic compound evolution in Cu/Sn solder joints under electromigration. Acta Materialia, 2013, 61, 7142-7154.	3.8	44
45	Towards stacking fault energy engineering in FCC high entropy alloys. Acta Materialia, 2022, 224, 117472.	3.8	44
46	Uncertainty Propagation Analysis of Computational Models in Laser Powder Bed Fusion Additive Manufacturing Using Polynomial Chaos Expansions. Journal of Manufacturing Science and Engineering, Transactions of the ASME, 2018, 140, .	1.3	41
47	Bayesian uncertainty quantification and information fusion in CALPHAD-based thermodynamic modeling. Acta Materialia, 2019, 164, 636-647.	3.8	41
48	Effect of ternary additions to structural properties of NiTi alloys. Computational Materials Science, 2016, 112, 347-355.	1.4	40
49	Machine Learning-Directed Navigation of Synthetic Design Space: A Statistical Learning Approach to Controlling the Synthesis of Perovskite Halide Nanoplatelets in the Quantum-Confined Regime. Chemistry of Materials, 2019, 31, 3281-3292.	3.2	40
50	Probing the entropy hypothesis in highly concentrated alloys. Acta Materialia, 2018, 148, 263-279.	3.8	39
51	Efficient machine-learning model for fast assessment of elastic properties of high-entropy alloys. Acta Materialia, 2022, 232, 117924.	3.8	39
52	Thermodynamic modelling of the Agâ€“Cuâ€“Ti ternary system. International Journal of Materials Research, 2011, 102, 286-297.	0.1	38
53	High-throughput combinatorial study of the effect of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>M</mml:mi></mml:math>site alloying on the solid solution behavior of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>M</mml:mi><mml:mn>2</mml:mn></mm phases. Physical Review B, 2016, 94, .	1.1	38
54	Formation and Growth of Intermetallic Compound Cu6Sn5 at Early Stages in Lead-Free Soldering. Journal of Electronic Materials, 2010, 39, 2574-2582.	1.0	37

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55	Finite-temperature elasticity of fcc Al: Atomistic simulations and ultrasonic measurements. Physical Review B, 2011, 84, .	1.1	37
56	Hydrogen sorption in orthorhombic Mg hydride at ultra-low temperature. International Journal of Hydrogen Energy, 2013, 38, 8328-8341.	3.8	36
57	Multivariate Calibration and Experimental Validation of a 3D Finite Element Thermal Model for Laser Powder Bed Fusion Metal Additive Manufacturing. Integrating Materials and Manufacturing Innovation, 2018, 7, 116-135.	1.2	36
58	Ab-initio aprroach to the electronic, structural, elastic, and finite-temperature thermodynamic properties of Ti2AX (Aâ€‰=â€‰Al or Ga and Xâ€‰=â€‰C or N). Journal of Applied Physics, 2011, 110, .	1.1	35
59	A data-driven machine learning approach to predicting stacking faulting energy in austenitic steels. Journal of Materials Science, 2017, 52, 11048-11076.	1.7	35
60	On the interfacial phase growth and vacancy evolution during accelerated electromigration in Cu/Sn/Cu microjoints. Acta Materialia, 2018, 160, 185-198.	3.8	35
61	Uncertainty Quantification and Propagation in Computational Materials Science and Simulation-Assisted Materials Design. Integrating Materials and Manufacturing Innovation, 2020, 9, 103-143.	1.2	35
62	Finite-temperature thermodynamic and vibrational properties of Alâ€“Niâ€“Y compounds via first-principles calculations. Acta Materialia, 2006, 54, 2291-2304.	3.8	34
63	Thermodynamic modeling of the Caâ€“Sn system based on finite temperature quantities from first-principles and experiment. Acta Materialia, 2006, 54, 4939-4951.	3.8	34
64	Prediction of the glass forming ability in Cuâ€“Zr binary and Cuâ€“Zrâ€“Ti ternary alloys. Intermetallics, 2008, 16, 27-33.	1.8	34
65	Modification of the thermodynamic model for the Mgâ€“Zr system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2005, 29, 230-238.	0.7	33
66	The Uâ€“Ti system: Strengths and weaknesses of the CALPHAD method. Journal of Nuclear Materials, 2011, 419, 177-185.	1.3	33
67	Multi-Information Source Fusion and Optimization to Realize ICME: Application to Dual-Phase Materials. Journal of Mechanical Design, Transactions of the ASME, 2018, 140, .	1.7	32
68	Experimental and computational study of the morphological evolution of intermetallic compound (Cu6Sn5) layers at the Cu/Sn interface under isothermal soldering conditions. Acta Materialia, 2012, 60, 5125-5134.	3.8	30
69	Strain-induced suppression of the miscibility gap in nanostructured Mg₂Siâ€“Mg₂Sn solid solutions. Journal of Materials Chemistry A, 2018, 6, 17559-17570.	5.2	30
70	Effect of configurational order on the magnetic characteristics of Co-Ni-Ga ferromagnetic shape memory alloys. Physical Review B, 2011, 84, .	1.1	29
71	Microstructural refinement in an ultra-high strength martensitic steel via equal channel angular pressing. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2018, 725, 57-64.	2.6	29
72	Investigation of the structural stability of Co2NiGa shape memory alloys via ab initio methods. Acta Materialia, 2010, 58, 5220-5231.	3.8	28

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73	The effect of electronic and magnetic valences on the martensitic transformation of CoNiGa shape memory alloys. Acta Materialia, 2012, 60, 3545-3558.	3.8	28
74	Bayesian Calibration and Uncertainty Quantification for a Physics-Based Precipitation Model of Nickelâ€“Titanium Shape-Memory Alloys. Journal of Manufacturing Science and Engineering, Transactions of the ASME, 2017, 139, .	1.3	28
75	Functionally Graded Materials through robotics-inspired path planning. Materials and Design, 2019, 182, 107975.	3.3	28
76	Bayesian optimization with adaptive surrogate models for automated experimental design. Npj Computational Materials, 2021, 7, .	3.5	27
77	Multiphase Field Simulations of Intermetallic Compound Growth During Lead-Free Soldering. Journal of Electronic Materials, 2009, 38, 2525-2533.	1.0	26
78	Computational investigation of intermetallic compounds (Cu6Sn5 and Cu3Sn) growth during solid-state aging process. Computational Materials Science, 2011, 50, 1692-1700.	1.4	26
79	Development of a kinetic model for bainitic isothermal transformation in transformation-induced plasticity steels. Acta Materialia, 2013, 61, 2884-2894.	3.8	26
80	Processing of novel pseudomorphic Cuâ€“Mo hierarchies in thin films. Materials Research Letters, 2019, 7, 1-11.	4.1	26
81	Phase constitution effect on the ductility of low alloy multiphase transformation induced plasticity steels. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2013, 569, 137-143.	2.6	25
82	Stabilization of bcc Mg in Thin Films at Ambient Pressure: Experimental Evidence andab initioCalculations. Materials Research Letters, 2013, 1, 161-167.	4.1	25
83	First-principles calculations of finite-temperature elastic properties of Ti2AlX (X=C or N). Computational Materials Science, 2013, 79, 296-302.	1.4	24
84	Properties and Decomposition of Heusler Alloys. Energy Technology, 2018, 6, 1478-1490.	1.8	24
85	Glassy Phonon Heralds a Strain Glass State in a Shape Memory Alloy. Physical Review Letters, 2018, 120, 245701.	2.9	24
86	Navigating the design space of inorganic materials synthesis using statistical methods and machine learning. Dalton Transactions, 2020, 49, 11480-11488.	1.6	24
87	Semi-supervised learning approaches to class assignment in ambiguous microstructures. Acta Materialia, 2020, 188, 49-62.	3.8	24
88	Prediction of processing maps for transient liquid phase diffusion bonding of Cu/Sn/Cu joints in microelectronics packaging. Microelectronics Reliability, 2014, 54, 1401-1411.	0.9	23
89	Uncertainty propagation in a multiscale CALPHAD-reinforced elastochemical phase-field model. Acta Materialia, 2020, 183, 452-470.	3.8	23
90	Atomic Hourglass and Thermometer Based on Diffusion of a Mobile Dopant in VO₂. Journal of the American Chemical Society, 2020, 142, 15513-15526.	6.6	23

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91	Thermodynamic analysis of two-stage heat treatment in TRIP steels. Acta Materialia, 2012, 60, 6120-6130.	3.8	22
92	Multi-objective materials bayesian optimization with active learning of design constraints: Design of ductile refractory multi-principal-element alloys. Acta Materialia, 2022, 236, 118133.	3.8	22
93	Mass transport and thermal stability of TiN/Al2O3/InGaAs nanofilms. Journal of Applied Physics, 2012, 112, .	1.1	21
94	Efficient use of multiple information sources in material design. Acta Materialia, 2019, 180, 260-271.	3.8	21
95	Experiment Design Frameworks for Accelerated Discovery of Targeted Materials Across Scales. Frontiers in Materials, 2019, 6, .	1.2	21
96	Structural and transport properties of epitaxial NaxCoO2 thin films. Applied Physics Letters, 2005, 87, 172104.	1.5	20
97	Diffusion of In and Ga in TiN/HfO2/InGaAs nanofilms. Journal of Applied Physics, 2013, 114, .	1.1	20
98	Does aluminum play well with others? Intrinsic Al-A alloying behavior in 211/312 MAX phases. Materials Research Letters, 2017, 5, 170-178.	4.1	20
99	Ab initioinvestigation of Ti<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Al(C,N) solid solutions. Physical Review B, 2011, 84, .	1.1	19
100	First-principles investigation of the Alâ€“Siâ€“Sr ternary system: Ground state determination and mechanical properties. Intermetallics, 2012, 21, 31-44.	1.8	19
101	Lattice vibrations boost demagnetization entropy in a shape-memory alloy. Physical Review B, 2015, 92, .	1.1	19
102	Metal cluster-deposited graphene as an adsorptive material for m-xylene. New Journal of Chemistry, 2015, 39, 9650-9658.	1.4	19
103	Computational Design of Gradient Paths in Additively Manufactured Functionally Graded Materials. Journal of Mechanical Design, Transactions of the ASME, 2018, 140, .	1.7	19
104	Magnetocaloric effects in Ni-Mn-Ga-Fe alloys using Monte Carlo simulations. Journal of Applied Physics, 2013, 113, 183904.	1.1	18
105	Efficiently exploiting process-structure-property relationships in material design by multi-information source fusion. Acta Materialia, 2021, 206, 116619.	3.8	18
106	Design of multifunctional supercapacitor electrodes using an informatics approach. Molecular Systems Design and Engineering, 2019, 4, 654-663.	1.7	17
107	On the complexity of solid-state diffusion in highly concentrated alloys and the sluggish diffusion core-effect. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2020, 68, 101713.	0.7	17
108	Adaptive active subspace-based efficient multifidelity materials design. Materials and Design, 2021, 209, 110001.	3.3	17

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109	On the stochastic phase stability of Ti2AlC-Cr2AlC. Scientific Reports, 2017, 7, 5138.	1.6	16
110	Exploration of the microstructure space in TiAlZrN ultra-hard nanostructured coatings. Acta Materialia, 2019, 174, 459-476.	3.8	16
111	Competing Interactions between Mesoscale Length-Scales, Order-Disorder, and Martensitic Transformation in Ferromagnetic Shape Memory Alloys. Acta Materialia, 2021, 206, 116616.	3.8	16
112	Phase transformations in equiatomic CuZr shape memory thin films analyzed by differential nanocalorimetry. Acta Materialia, 2018, 159, 320-331.	3.8	15
113	Design of alumina-forming austenitic stainless steel using genetic algorithms. Materials and Design, 2020, 186, 108198.	3.3	15
114	The effect of chemical disorder on defect formation and migration in disordered max phases. Acta Materialia, 2020, 184, 50-58.	3.8	15
115	Materials Design Through Batch Bayesian Optimization with Multisource Information Fusion. Jom, 2020, 72, 4431-4443.	0.9	15
116	Defect structures and ternary lattice site preference of the B2 phase in the Alâ€“Niâ€“Ru system. Acta Materialia, 2007, 55, 4781-4787.	3.8	14
117	Thermodynamic remodeling of the Coâ€“Ga system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2010, 34, 189-195.	0.7	14
118	Uncertainty analysis of microsegregation during laser powder bed fusion. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 034002.	0.8	14
119	Uncertainty quantification and propagation in CALPHAD modeling. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 034003.	0.8	14
120	Investigation of the discontinuous precipitation of U-Nb alloys via thermodynamic analysis and phase-field modeling. Computational Materials Science, 2020, 175, 109573.	1.4	13
121	High-throughput reaction engineering to assess the oxidation stability of MAX phases. Npj Computational Materials, 2021, 7, .	3.5	13
122	Machine-learning enabled thermodynamic model for the design of new rare-earth compounds. Acta Materialia, 2022, 229, 117759.	3.8	13
123	Open source software for materials and process modeling. Jom, 2008, 60, 32-39.	0.9	12
124	An inverse design framework for prescribing precipitation heat treatments from a target microstructure. Materials and Design, 2016, 107, 7-17.	3.3	12
125	Uncertainty quantification of the parameters and predictions of a phenomenological constitutive model for thermally induced phase transformation in Niâ€“Ti shape memory alloys. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 034001.	0.8	12
126	Martensitic Transformation in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:msub><mml:mrow><mml:mi>Fe</mml:mi></mml:mrow><mml:mrow><mml:mi>x</mml:mi></mml:mrow> Physical Review Letters, 2021, 127, 115704.	2.9	12

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127	Thermodynamics, lattice stability and defect structure of strontium silicides via first-principles calculations. Journal of Alloys and Compounds, 2009, 484, 822-831.	2.8	11
128	Stability analysis of the martensitic phase transformation in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Co</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> alloy. Physical Review B, 2015, 92, .	1.2	11
129	Probing Structural and Magnetic Instabilities and Hysteresis in Heuslers by Density Functional Theory Calculations. Physica Status Solidi (B): Basic Research, 2018, 255, 1700296.	0.7	11
130	Interdisciplinary Research on Designing Engineering Material Systems: Results From a National Science Foundation Workshop. Journal of Mechanical Design, Transactions of the ASME, 2018, 140, .	1.7	11
131	On the importance of microstructure information in materials design: PSP vs PP. Acta Materialia, 2022, 223, 117471.	3.8	11
132	Thermodynamic modeling of the Siâ€“Sr system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2009, 33, 550-556.	0.7	10
133	Ab-initio calculations of the elastic and finite-temperature thermodynamic properties of niobium- and magnesium hydrides. International Journal of Hydrogen Energy, 2014, 39, 15530-15539.	3.8	10
134	On the fast kinetics of B2â€“L21 ordering in Ni-Co-Mn-In metamagnetic shape memory alloys. Journal of Alloys and Compounds, 2019, 781, 479-489.	2.8	10
135	A proof of concept: Thermodynamics of aluminum â€“ transition metal highly concentrated alloys. Journal of Alloys and Compounds, 2019, 781, 595-605.	2.8	10
136	Nucleation-controlled hysteresis in unstrained hydrothermal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">V</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> particles. Physical Review Materials, 2018, 2, .	0.9	10
137	Microstructure classification in the unsupervised context. Acta Materialia, 2022, 223, 117434.	3.8	10
138	Accelerated materials design using batch Bayesian optimization: A case study for solving the inverse problem from materials microstructure to process specification. Computational Materials Science, 2022, 210, 111417.	1.4	10
139	A first-principles approach to transition states of diffusion. Journal of Physics Condensed Matter, 2012, 24, 305402.	0.7	9
140	Ab-initio investigation of the finite-temperatures structural, elastic, and thermodynamic properties of Ti3AlC2 and Ti3SiC2. Computational Materials Science, 2016, 124, 420-427.	1.4	9
141	Phase Field Modeling of Joint Formation During Isothermal Solidification in 3DIC Micro Packaging. Journal of Phase Equilibria and Diffusion, 2016, 37, 469-480.	0.5	9
142	A Constraint Satisfaction Algorithm for the Generalized Inverse Phase Stability Problem. Journal of Mechanical Design, Transactions of the ASME, 2017, 139, .	1.7	9
143	Nanocalorimetry and ab initio study of ternary elements in CuZr-based shape memory alloy. Acta Materialia, 2020, 182, 29-38.	3.8	9
144	Bayesian probabilistic prediction of precipitation behavior in Ni-Ti shape memory alloys. Computational Materials Science, 2020, 172, 109334.	1.4	9

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145	An efficient framework for printability assessment in Laser Powder Bed Fusion metal additive manufacturing. Additive Manufacturing, 2021, 46, 102018.	1.7	9
146	Thermodynamic study of the Npâ€“Zr system. Journal of Nuclear Materials, 2011, 409, 1-8.	1.3	8
147	The Inverse Phase Stability Problem as a Constraint Satisfaction Problem: Application to Materials Design. Jom, 2016, 68, 1385-1395.	0.9	8
148	Effects of composition and crystallographic ordering on the ferromagnetic transition in Ni Co Mn In magnetic shape memoryÂalloys. Acta Materialia, 2019, 166, 630-637.	3.8	8
149	Review: additive manufacturing of pure tungsten and tungsten-based alloys. Journal of Materials Science, 2022, 57, 9769-9806.	1.7	8
150	Predicting Van der Waals Heterostructures by a Combined Machine Learning and Density Functional Theory Approach. ACS Applied Materials & Interfaces, 2022, 14, 25907-25919.	4.0	8
151	Data-Enabled Discovery and Design of Energy Materials (D3EM): Structure of An Interdisciplinary Materials Design Graduate Program. MRS Advances, 2017, 2, 1693-1698.	0.5	7
152	Impact of particle arrays on phase separation composition patterns. Journal of Chemical Physics, 2020, 152, 224902.	1.2	7
153	Laser-based additive manufacturing of a binary Ni-5â€‰wt.%Nb alloy. Journal of Manufacturing Processes, 2021, 62, 720-728.	2.8	7
154	Effect of heat treatments on the microstructure and mechanical properties of an ultra-high strength martensitic steel fabricated via laser powder bed fusion additive manufacturing. Additive Manufacturing, 2021, 47, 102255.	1.7	7
155	On the limitations of the DFT+U approach to energetics of actinides. Computational Materials Science, 2012, 59, 48-56.	1.4	6
156	Firstâ€Principles Characterization of Equilibrium Vacancy Concentration in Metamagnetic Shape Memory Alloys: An Example of Ni₂MnGa. Physica Status Solidi (B): Basic Research, 2018, 255, 1700523.	0.7	6
157	Phase-Field Study of Thermomigration in 3-D IC Micro Interconnects. IEEE Transactions on Components, Packaging and Manufacturing Technology, 2020, 10, 1466-1473.	1.4	6
158	Metric-driven search for structurally stable inorganic compounds. Acta Materialia, 2021, 202, 437-447.	3.8	6
159	A printability assessment framework for fabricating low variability nickel-niobium parts using laser powder bed fusion additive manufacturing. Rapid Prototyping Journal, 2021, 27, 1737-1748.	1.6	6
160	Computational Investigation of the Evolution of Intermetallic Compounds Affected by Microvoids During the Solid-State Aging Process in the Cu-Sn System. Journal of Electronic Materials, 2013, 42, 999-1009.	1.0	5
161	Confinement Effects on Evolution of Intermetallic Compounds During Metallurgical Joint Formation. Journal of Electronic Materials, 2014, 43, 2510-2520.	1.0	5
162	Describing the deformation behaviour of TRIP and dual phase steels employing an irreversible thermodynamics formulation. Materials Science and Technology, 2015, 31, 1658-1663.	0.8	5

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163	Study of the Isothermal Oxidation Process and Phase Transformations in B2-(Ni,Pt)Al/RENE-N5 System. Metals, 2016, 6, 208.	1.0	5
164	Out-of-plane ordering in quaternary MAX alloys: an alloy theoretic perspective. Materials Research Letters, 2018, 6, 1-12.	4.1	5
165	Microstructure-Based Modeling of the Effect of Inclusion on the Bendability of Advanced High Strength Dual-Phase Steels. Metals, 2021, 11, 431.	1.0	5
166	A Top-Down Characterization of NiTi Single-Crystal Inelastic Properties within Confidence Bounds through Bayesian Inference. Shape Memory and Superelasticity, 2021, 7, 50-64.	1.1	5
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