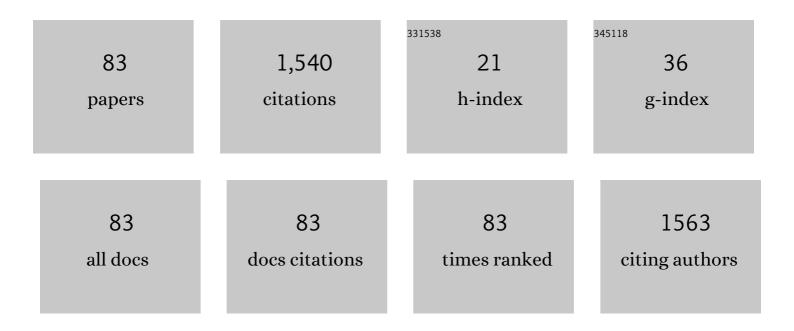
List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	The alloying effects of Ge and Si on thermal stability and crystallization behavior of Al-Y binary amorphous alloys. Journal of Non-Crystalline Solids, 2022, 575, 121197.	1.5	2
2	Defect-mediated crystal growth from deeply undercooled melts. Computational Materials Science, 2022, 201, 110861.	1.4	3
3	Short to medium range order and atomic dynamic property within the surface of nanoscale metallic glasses revealed by molecular dynamics simulations. Journal of Non-Crystalline Solids, 2022, 578, 121348.	1.5	5
4	First-Principles Investigation of the Interfacial Stability, Precipitate Formation, and Mechanical Behavior of Al3Li/Al3Zr/Al Interfaces. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2022, 53, 1308-1321.	1.1	3
5	Composition dependence in glass-forming ability of Cu–Ag binary alloys. Acta Materialia, 2022, 235, 118059.	3.8	4
6	Pressure effects on the dynamics and glass formation of Cu-Ag eutectic melt. Journal of Non-Crystalline Solids, 2022, 594, 121800.	1.5	0
7	Intermediate structural evolution preceding growing BCC crystal interface in deeply undercooled monatomic metallic liquids. Acta Materialia, 2021, 202, 387-398.	3.8	10
8	Solid-solution strengthening effects in binary Ni-based alloys evaluated by high-throughput calculations. Materials and Design, 2021, 198, 109359.	3.3	24
9	Thermal neutron scattering properties of Bismuth crystal filter. Journal of Nuclear Science and Technology, 2021, 58, 704-713.	0.7	Ο
10	Balancing crystallization rate in a mixed Sn–Pb perovskite film for efficient and stable perovskite solar cells of more than 20% efficiency. Journal of Materials Chemistry A, 2021, 9, 17830-17840.	5.2	51
11	Tuning the Interfacial Dipole Moment of Spacer Cations for Charge Extraction in Efficient and Ultrastable Perovskite Solar Cells. Journal of Physical Chemistry C, 2021, 125, 1256-1268.	1.5	56
12	Abnormal dynamic behavior and structural origin of Cu-Ag eutectic melt. Acta Materialia, 2021, 207, 116705.	3.8	3
13	Temperature dependent size effects on crystal growth of nanorods revealed by molecular dynamics simulations. Journal of Applied Physics, 2021, 129, 194302.	1.1	Ο
14	A generally reliable model for composition-dependent lattice constants of substitutional solid solutions. Acta Materialia, 2021, 211, 116865.	3.8	9
15	Influences of Si addition on the thermal stability and crystallization behavior of Al-Y binary amorphous alloys. Journal of Alloys and Compounds, 2021, 873, 159816.	2.8	2
16	Effects of alloying elements on the Ni/Ni3Al interface strength and vacancy diffusion behavior. Journal of Applied Physics, 2020, 128, .	1.1	7
17	Unusual internal friction and its size dependence in nanoscale metallic glasses. Journal of Applied Physics, 2020, 128, .	1.1	2
18	Correlations among atomic mobility, microstructure and local stress of shear bands and necking regions in notched Cu50Zr50 metallic glasses. Journal of Applied Physics, 2019, 126, .	1.1	4

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19	First principles investigation of the vacancy-mediated impurity diffusion in dilute Zr-X (X = Sc, Y, Ce) alloys. Nuclear Instruments & Methods in Physics Research B, 2019, 453, 75-78.	0.6	5
20	The atomic packing structure of Al-(TM)-Y metallic glasses. Intermetallics, 2019, 111, 106505.	1.8	7
21	Influence of substitution of La by Gd on crystallization behavior of Al-Ni-La metallic glasses. Journal of Alloys and Compounds, 2019, 790, 626-632.	2.8	11
22	Novel pyrochlore-type La2Zr2O7: Eu3+ red phosphors: Synthesis, structural, luminescence properties and theoretical calculation. Dyes and Pigments, 2018, 157, 47-54.	2.0	77
23	Predicting Shear Transformation Events in Metallic Glasses. Physical Review Letters, 2018, 120, 125503.	2.9	52
24	Effect of notch depth on the mechanical behavior of Cu50Zr50 metallic glasses revealed by molecular dynamics simulations. Intermetallics, 2018, 93, 303-311.	1.8	8
25	On the Optimal Glass-Forming Composition of Al–Co–Y Amorphous Alloys. Materials Transactions, 2018, 59, 1545-1550.	0.4	1
26	Solid-liquid interfacial free energy and its anisotropy in the Cu-Ni binary system investigated by molecular dynamics simulations. Journal of Alloys and Compounds, 2017, 708, 1073-1080.	2.8	24
27	Strain-dependent activation energy of shear transformation in metallic glasses. Physical Review B, 2017, 95, .	1.1	18
28	A comparative study on local atomic configurations characterized by cluster-type-index method and Voronoi polyhedron method. Computational Materials Science, 2016, 123, 214-223.	1.4	35
29	Impact toughness scattering of bainitic steel in the ductile-brittle transition temperature region. Journal Wuhan University of Technology, Materials Science Edition, 2016, 31, 636-643.	0.4	3
30	Atomistic characterization of solid-liquid interfaces in the Cu-Ni binary alloy system. Computational Materials Science, 2016, 125, 72-81.	1.4	16
31	Size effects in Cu50Zr50 metallic glass films revealed by molecular dynamics simulations. Journal of Alloys and Compounds, 2016, 688, 88-95.	2.8	43
32	Glassâ€Forming Ability and Crystallization Behavior of Al <sub>86</sub> Ni <sub>9</sub> La <sub>5</sub> Metallic Glass with Si Addition. Advanced Engineering Materials, 2016, 18, 972-977.	1.6	17
33	Effect of Bainitic Packet Size Distribution on Impact Toughness and its Scattering in the Ductile-Brittle Transition Temperature Region of Q&T Mn-Ni-Mo Bainitic Steels. Steel Research International, 2016, 87, 165-172.	1.0	8
34	Influence of mutual substitution between La and Gd on the glass-forming ability of Al–Ni–La–Gd alloys. Journal of Alloys and Compounds, 2015, 628, 245-250.	2.8	6
35	Glass forming ability of Al–Ni–La alloys with Si addition. Journal of Alloys and Compounds, 2015, 650, 578-583.	2.8	9
36	Abnormal crystallization behavior of an (Al86Ni9La5)98Si2 amorphous alloy. Materials Letters, 2015, 159, 403-405.	1.3	5

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37	Heterogeneous nucleation at inoculant particles in a glass forming alloy: An ab initio molecular dynamics investigation of interfacial properties and local chemical bonding. Computational Materials Science, 2015, 108, 94-102.	1.4	10
38	Atomic structure and thermal stability of interfaces between metallic glass and embedding nano-crystallites revealed by molecular dynamics simulations. Journal of Alloys and Compounds, 2015, 647, 331-337.	2.8	10
39	Orientation dependences of atomic structures in chemically heterogeneous Cu50Ta50/Ta glass-crystal interfaces. Journal of Applied Physics, 2015, 117, 015303.	1.1	4
40	Structural and dynamical properties of heterogeneous solid–liquid Ta–Cu interfaces: A molecular dynamics study. Computational Materials Science, 2014, 86, 64-72.	1.4	15
41	Pseudo-elasticity and ultra-high recoverable strain in cobalt nanowire: A molecular dynamics study. Scripta Materialia, 2013, 68, 191-194.	2.6	7
42	Microstructure and Mechanical Properties of Cu–Zr–Al Bulk Metallic Glass with Addition of Co. Materials Transactions, 2013, 54, 286-290.	0.4	12
43	Dynamical stability of iron under high-temperature and high-pressure conditions. Europhysics Letters, 2012, 97, 56004.	0.7	14
44	Glass forming ability and primary crystallization behavior of Al–Ni–Ce alloys. Intermetallics, 2012, 24, 1-6.	1.8	18
45	Correlation between mechanical behavior and glass forming ability of Zr–Cu metallic glasses. Intermetallics, 2011, 19, 1032-1035.	1.8	31
46	Rolling-induced microstructure change in Zr65Al7.5Ni10Cu12.5Ag5 bulk metallic glass. Science Bulletin, 2011, 56, 3948-3951.	1.7	3
47	An improved version of the Green's function molecular dynamics method. Computer Physics Communications, 2011, 182, 540-541.	3.0	14
48	Phonon dispersion measured directly from molecular dynamics simulations. Computer Physics Communications, 2011, 182, 2201-2207.	3.0	217
49	Quantitative results for square gradient models of fluids. Europhysics Letters, 2011, 93, 50004.	0.7	4
50	The crucial role of chemical detail for slip-boundary conditions: molecular dynamics simulations of linear oligomers between sliding aluminum surfaces. Modelling and Simulation in Materials Science and Engineering, 2010, 18, 034004.	0.8	24
51	Implementation of Green's function molecular dynamics: An extension to LAMMPS. Computer Physics Communications, 2009, 180, 1004-1010.	3.0	56
52	Non-bonded force field for the interaction between metals and organic molecules: a case study of olefins on aluminum. Physical Chemistry Chemical Physics, 2009, 11, 10195.	1.3	14
53	Surface diffusion coefficients: Substrate dynamics matters. Physical Review B, 2008, 77, .	1.1	30
54	Structure and energetics ofcâ^'Siâ^•aâ^'SiO2systems: Planar interfaces and embedded Si nanocrystals. Physical Review B, 2008, 77, .	1.1	15

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55	Distinct magnetic states of metastable fcc structured Fe and Fe–Cu alloys studied by ab initio calculations. Journal of Alloys and Compounds, 2006, 414, 36-41.	2.8	25
56	Structure stability and magnetic properties of the Ni–Ru system studied by ab initio and molecular dynamics calculations together with ion beam mixing. Acta Materialia, 2006, 54, 3375-3381.	3.8	22
57	Transition state theory of the preexponential factors for self-diffusion on Cu, Ag, and Ni surfaces. Physical Review B, 2006, 74, .	1.1	44
58	Orientation and Composition Dependences of the Surface Energy and Work Function Observed by First-Principles Calculation for the Mo–Hf System. Journal of the Physical Society of Japan, 2005, 74, 1766-1771.	0.7	9
59	Stability of the Metastable Phases in the Co–Ta System Studied byab initioand Thermodynamic Calculations Together with Ion-Beam-Mixing Experiment. Journal of the Physical Society of Japan, 2005, 74, 2501-2505.	0.7	11
60	Calculation of ferromagnetic states in metastable bcc and hcp Ni by projector-augmented wave method. Journal of Applied Physics, 2005, 97, 106107.	1.1	27
61	Metastable Phase Selection of an Immiscible Au–W System Studied byab initioCalculation, Molecular Dynamics Simulation and Ion-Beam Mixing. Japanese Journal of Applied Physics, 2004, 43, 7648-7653.	0.8	1
62	Structural Stability and the Correlation of Lattice Constant versus Tantalum Concentration of the Ag-Based Fcc Solid Solutions Studied by Molecular Dynamics Simulation. Japanese Journal of Applied Physics, 2004, 43, 2589-2593.	0.8	3
63	Comparative study of metastable phase formation in the immiscible Cu–W system byab initiocalculation andn-body potential. Journal of Physics Condensed Matter, 2004, 16, 5251-5258.	0.7	18
64	Metastability of an immiscible Cu-Mo system calculated from first-principles and a derivedn-body potential. Physical Review B, 2004, 69, .	1.1	18
65	Structural stability and magnetic properties of metastable Fe-Cu alloys studied byab initiocalculations and molecular dynamics simulations. Physical Review B, 2004, 69, .	1.1	17
66	Correlation of magnetic moment versus spacing distance of metastable fcc structured iron. Applied Physics Letters, 2004, 84, 3627-3629.	1.5	46
67	Structural transition and glass-forming ability of the Ni–Hf system studied by molecular dynamics simulation. Journal of Materials Research, 2004, 19, 3547-3555.	1.2	16
68	Glass-forming ability determined from inter-atomic potentials for some miscible/immiscible binary metal systems. Journal of Materials Science, 2004, 39, 5067-5070.	1.7	1
69	Proposed Definition of Microchemical Inhomogeneity and Application To Characterize Some Selected Miscible/Immiscible Binary Metal Systems. Journal of Physical Chemistry B, 2004, 108, 16071-16076.	1.2	20
70	Structural phase transitions in the Cu-based Cu–V solid solutions studied by molecular dynamics simulation. Journal of Alloys and Compounds, 2004, 366, 205-212.	2.8	6
71	Ab initio calculation to predict the possible nonequilibrium A3B and AB3 states in the Co–Mo system. Solid State Communications, 2003, 125, 435-437.	0.9	4
72	Metastable phase formation in an immiscible Cu-Ta system studied by ion-beam mixing, ab initio calculation, and molecular dynamics simulation. Acta Materialia, 2003, 51, 3885-3893.	3.8	17

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73	Amorphous Alloy Formation in Immiscible Cu-Ta and Cu-W Systems by Atomistic Modeling and Ion-Beam Mixing. Materials Research Society Symposia Proceedings, 2003, 806, 220.	0.1	6
74	Prediction of metastable phase formation in an immiscible Cu–Cr system from interatomic potential and ab initio calculation. Journal of Materials Research, 2003, 18, 2300-2303.	1.2	3
75	Glass-forming ability determined by ann-body potential in a highly immiscible Cu-W system through molecular dynamics simulations. Physical Review B, 2003, 68, .	1.1	20
76	Construction of an N-Body Cu–Ta Potential and Study of Interfacial Behavior between Immiscible Cu and Ta through Molecular Dynamics Simulation. Journal of the Physical Society of Japan, 2003, 72, 5-8.	0.7	5
77	Construction of an Embedded-Atom Potential for an Immiscible Cu–V System. Journal of the Physical Society of Japan, 2003, 72, 464-467.	0.7	3
78	Atomistic modeling of solid-state amorphization in an immiscible Cu-Ta system. Physical Review B, 2002, 66, .	1.1	56
79	Formation of a dodecagonal phase in the nano-sized Ag-Pt multilayers upon solid-state reaction. Journal of Physics Condensed Matter, 2002, 14, 1-5.	0.7	56
80	Interfacial Reaction of W/Cu Examined by an n-body Potential through Molecular Dynamics Simulations. Japanese Journal of Applied Physics, 2002, 41, 4503-4508.	0.8	11
81	Prediction of Possible Metastable Alloy Phases in an Equilibrium Immiscible Y–Mo System by ab initio Calculation. Journal of Materials Research, 2002, 17, 528-531.	1.2	3
82	Ab initio Calculation to Predict Possible Non-Equilibrium Solid Phases in an Immiscible Y–Nb System. Journal of the Physical Society of Japan, 2002, 71, 141-143.	0.7	14
83	Correlation of lattice constant versus tungsten concentration of the Ni-based solid solution examined by molecular dynamics simulation. Journal of Alloys and Compounds, 2002, 337, 143-147.	2.8	30