Ling-Ti Kong

List of Publications by Year
in descending order

83 papers	1,540 citations	331538 21 h-index	345118 36 g-index
83 all docs	83 docs citations	83 times ranked	1563 citing authors

#	Article	IF	Citations
1	Phonon dispersion measured directly from molecular dynamics simulations. Computer Physics Communications, 2011, 182, 2201-2207.	3.0	217
2	Novel pyrochlore-type La2Zr2O7: Eu3+ red phosphors: Synthesis, structural, luminescence properties and theoretical calculation. Dyes and Pigments, 2018, 157, 47-54.	2.0	77
3	Atomistic modeling of solid-state amorphization in an immiscible Cu-Ta system. Physical Review B, 2002, 66, .	1.1	56
4	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
5	Implementation of Green's function molecular dynamics: An extension to LAMMPS. Computer Physics Communications, 2009, 180, 1004-1010.	3.0	56
6	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
7	Predicting Shear Transformation Events in Metallic Glasses. Physical Review Letters, 2018, 120, 125503.	2.9	52
8	Balancing crystallization rate in a mixed Snâ€“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
9	Correlation of magnetic moment versus spacing distance of metastable fcc structured iron. Applied Physics Letters, 2004, 84, 3627-3629.	1.5	46
10	Transition state theory of the preexponential factors for self-diffusion on Cu, Ag, and Ni surfaces. Physical Review B, 2006, 74, .	1.1	44
11	Size effects in Cu50Zr50 metallic glass films revealed by molecular dynamics simulations. Journal of Alloys and Compounds, 2016, 688, 88-95.	2.8	43
12	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
13	Correlation between mechanical behavior and glass forming ability of Zrâ€“Cu metallic glasses. Intermetallics, 2011, 19, 1032-1035.	1.8	31
14	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
15	Surface diffusion coefficients: Substrate dynamics matters. Physical Review B, 2008, 77, .	1.1	30
16	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
17	Distinct magnetic states of metastable fcc structured Fe and Feâ€“Cu alloys studied by ab initio calculations. Journal of Alloys and Compounds, 2006, 414, 36-41.	2.8	25
18	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

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19	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
20	Solid-solution strengthening effects in binary Ni-based alloys evaluated by high-throughput calculations. Materials and Design, 2021, 198, 109359.	3.3	24
21	Structure stability and magnetic properties of the Niâ€“Ru system studied by ab initio and molecular dynamics calculations together with ion beam mixing. Acta Materialia, 2006, 54, 3375-3381.	3.8	22
22	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
23	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
24	Comparative study of metastable phase formation in the immiscible Cuâ€“W system byab initiocalculation andn-body potential. Journal of Physics Condensed Matter, 2004, 16, 5251-5258.	0.7	18
25	Metastability of an immiscible Cu-Mo system calculated from first-principles and a derivedn-body potential. Physical Review B, 2004, 69, .	1.1	18
26	Glass forming ability and primary crystallization behavior of Alâ€“Niâ€“Ce alloys. Intermetallics, 2012, 24, 1-6.	1.8	18
27	Strain-dependent activation energy of shear transformation in metallic glasses. Physical Review B, 2017, 95, .	1.1	18
28	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
29	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
30	Glassâ€Forming Ability and Crystallization Behavior of Al₈₆Ni₉La₅ Metallic Glass with Si Addition. Advanced Engineering Materials, 2016, 18, 972-977.	1.6	17
31	Structural transition and glass-forming ability of the Niâ€“Hf system studied by molecular dynamics simulation. Journal of Materials Research, 2004, 19, 3547-3555.	1.2	16
32	Atomistic characterization of solid-liquid interfaces in the Cu-Ni binary alloy system. Computational Materials Science, 2016, 125, 72-81.	1.4	16
33	Structure and energetics ofcâ^'Siâ^•aâ^'SiO2systems: Planar interfaces and embedded Si nanocrystals. Physical Review B, 2008, 77, .	1.1	15
34	Structural and dynamical properties of heterogeneous solidâ€“liquid Taâ€“Cu interfaces: A molecular dynamics study. Computational Materials Science, 2014, 86, 64-72.	1.4	15
35	Ab initio Calculation to Predict Possible Non-Equilibrium Solid Phases in an Immiscible Yâ€“Nb System. Journal of the Physical Society of Japan, 2002, 71, 141-143.	0.7	14
36	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

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37	An improved version of the Green's function molecular dynamics method. Computer Physics Communications, 2011, 182, 540-541.	3.0	14
38	Dynamical stability of iron under high-temperature and high-pressure conditions. Europhysics Letters, 2012, 97, 56004.	0.7	14
39	Microstructure and Mechanical Properties of Cu–Zr–Al Bulk Metallic Glass with Addition of Co. Materials Transactions, 2013, 54, 286-290.	0.4	12
40	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
41	Stability of the Metastable Phases in the Coâ€“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
42	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
43	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
44	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
45	Intermediate structural evolution preceding growing BCC crystal interface in deeply undercooled monatomic metallic liquids. Acta Materialia, 2021, 202, 387-398.	3.8	10
46	Orientation and Composition Dependences of the Surface Energy and Work Function Observed by First-Principles Calculation for the Moâ€“Hf System. Journal of the Physical Society of Japan, 2005, 74, 1766-1771.	0.7	9
47	Glass forming ability of Alâ€“Niâ€“La alloys with Si addition. Journal of Alloys and Compounds, 2015, 650, 578-583.	2.8	9
48	A generally reliable model for composition-dependent lattice constants of substitutional solid solutions. Acta Materialia, 2021, 211, 116865.	3.8	9
49	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
50	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
51	Pseudo-elasticity and ultra-high recoverable strain in cobalt nanowire: A molecular dynamics study. Scripta Materialia, 2013, 68, 191-194.	2.6	7
52	The atomic packing structure of Al-(TM)-Y metallic glasses. Intermetallics, 2019, 111, 106505.	1.8	7
53	Effects of alloying elements on the Ni/Ni3Al interface strength and vacancy diffusion behavior. Journal of Applied Physics, 2020, 128, .	1.1	7
54	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

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55	Structural phase transitions in the Cu-based Cuâ€“V solid solutions studied by molecular dynamics simulation. Journal of Alloys and Compounds, 2004, 366, 205-212.	2.8	6
56	Influence of mutual substitution between La and Gd on the glass-forming ability of Alâ€“Niâ€“Laâ€“Gd alloys. Journal of Alloys and Compounds, 2015, 628, 245-250.	2.8	6
57	Construction of an N-Body Cuâ€“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
58	Abnormal crystallization behavior of an (Al86Ni9La5)98Si2 amorphous alloy. Materials Letters, 2015, 159, 403-405.	1.3	5
59	First principles investigation of the vacancy-mediated impurity diffusion in dilute Zr-X (Xâ€¯=â€¯Sc, Y, Ce) alloys. Nuclear Instruments & Methods in Physics Research B, 2019, 453, 75-78.	0.6	5
60	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
61	Ab initio calculation to predict the possible nonequilibrium A3B and AB3 states in the Coâ€“Mo system. Solid State Communications, 2003, 125, 435-437.	0.9	4
62	Quantitative results for square gradient models of fluids. Europhysics Letters, 2011, 93, 50004.	0.7	4
63	Orientation dependences of atomic structures in chemically heterogeneous Cu50Ta50/Ta glass-crystal interfaces. Journal of Applied Physics, 2015, 117, 015303.	1.1	4
64	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
65	Composition dependence in glass-forming ability of Cuâ€“Ag binary alloys. Acta Materialia, 2022, 235, 118059.	3.8	4
66	Prediction of Possible Metastable Alloy Phases in an Equilibrium Immiscible Yâ€“Mo System by ab initio Calculation. Journal of Materials Research, 2002, 17, 528-531.	1.2	3
67	Prediction of metastable phase formation in an immiscible Cuâ€“Cr system from interatomic potential and ab initio calculation. Journal of Materials Research, 2003, 18, 2300-2303.	1.2	3
68	Construction of an Embedded-Atom Potential for an Immiscible Cuâ€“V System. Journal of the Physical Society of Japan, 2003, 72, 464-467.	0.7	3
69	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
70	Rolling-induced microstructure change in Zr65Al7.5Ni10Cu12.5Ag5 bulk metallic glass. Science Bulletin, 2011, 56, 3948-3951.	1.7	3
71	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
72	Abnormal dynamic behavior and structural origin of Cu-Ag eutectic melt. Acta Materialia, 2021, 207, 116705.	3.8	3

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73	Defect-mediated crystal growth from deeply undercooled melts. Computational Materials Science, 2022, 201, 110861.	1.4	3
74	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
75	Unusual internal friction and its size dependence in nanoscale metallic glasses. Journal of Applied Physics, 2020, 128, .	1.1	2
76	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
77	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
78	Metastable Phase Selection of an Immiscible Auâ€“W System Studied byab initioCalculation, Molecular Dynamics Simulation and Ion-Beam Mixing. Japanese Journal of Applied Physics, 2004, 43, 7648-7653.	0.8	1
79	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
80	On the Optimal Glass-Forming Composition of Alâ€“Coâ€“Y Amorphous Alloys. Materials Transactions, 2018, 59, 1545-1550.	0.4	1
81	Thermal neutron scattering properties of Bismuth crystal filter. Journal of Nuclear Science and Technology, 2021, 58, 704-713.	0.7	0
82	Temperature dependent size effects on crystal growth of nanorods revealed by molecular dynamics simulations. Journal of Applied Physics, 2021, 129, 194302.	1.1	0
83	Pressure effects on the dynamics and glass formation of Cu-Ag eutectic melt. Journal of Non-Crystalline Solids, 2022, 594, 121800.	1.5	0