Jian-Bo Liu

List of Publications by Year
in descending order

67	1,183	448610 19	466096 32
papers	citations	h-index	g-index

68	68	68	2336
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Improved hydrothermal durability of Cu-SSZ-13 NH3-SCR catalyst by surface Al modification: Affinity and passivation. Journal of Catalysis, 2022, 405, 199-211.	3.1	28
2	Construction of Al-Mg-Zn Interatomic Potential and the Prediction of Favored Glass Formation Compositions and Associated Driving Forces. Materials, 2022, 15, 2062.	1.3	3
3	Optical/electrical properties of RENiO3 (RE = Pr, Nd, Sm, Gd, Dy, Ho, Er, Y and Lu) with intrinsic point defects: A first-principles study. Journal of Solid State Chemistry, 2022, 312, 123162.	1.4	2
4	Exotic Structural and Optoelectronic Properties of Layered Halide Double Perovskite Polymorphs. Advanced Functional Materials, 2021, 31, 2008620.	7.8	5
5	Insights into the Electrochemical Stability and Lithium Conductivity of Li₄MS₄ (M = Si, Ge, and Sn). ACS Applied Materials & Interfaces, 2021, 13, 22438-22447.	4.0	7
6	Electronic structure and stability of the (0 0 1) surface of halide double perovskite Cs2AgBiBr6. Applied Surface Science, 2021, 570, 151223.	3.1	1
7	Comparison of interatomic potentials on crack propagation properties in bcc iron. International Journal of Pressure Vessels and Piping, 2021, 194, 104524.	1.2	2
8	Alloy engineering in mixed Snâ€“Ge perovskites for photovoltaic application. Journal of Materials Chemistry A, 2021, 9, 6955-6961.	5.2	14
9	Lithium superionic conduction in Î±-Li10P4N10: A promising inorganic solid electrolyte candidate. Journal of Power Sources, 2020, 477, 228744.	4.0	3
10	Balancing strength and ductility of cylindrical-shaped Cu64Zr36 nanoglass via embedded Cu nanocrystals. Journal of Non-Crystalline Solids, 2020, 544, 120211.	1.5	3
11	Response to Comment on â€œPrediction of Novel pâ€Type Transparent Conductors in Layered Double Perovskites: A Firstâ€Principles Studyâ€• Advanced Functional Materials, 2020, 30, 2003149.	7.8	5
12	Enhanced surface binding energy regulates uniform potassium deposition for stable potassium metal anodes. Journal of Materials Chemistry A, 2020, 8, 5671-5678.	5.2	54
13	Relationships between copper speciation and BrÃ¸nsted acidity evolution over Cu-SSZ-13 during hydrothermal aging. Applied Catalysis A: General, 2020, 602, 117650.	2.2	38
14	Atomistic design favored compositions and atomic-level structure of Mgâ€“Caâ€“Ag ternary metallic glasses. AIP Advances, 2019, 9, .	0.6	3
15	Defect Engineering of Grain Boundaries in Leadâ€Free Halide Double Perovskites for Better Optoelectronic Performance. Advanced Functional Materials, 2019, 29, 1805870.	7.8	30
16	Green Emission Induced by Intrinsic Defects in All-Inorganic Perovskite CsPb₂Br₅. Journal of Physical Chemistry Letters, 2019, 10, 6118-6123.	2.1	28
17	First principles study of H2O adsorption on U2Ti (1â€¯1â€¯0) surface. Nuclear Instruments & Methods in Physics Research B, 2019, 457, 63-71.	0.6	5
18	Low-Temperature Solid-State Ion-Exchange Method for Preparing Cu-SSZ-13 Selective Catalytic Reduction Catalyst. ACS Catalysis, 2019, 9, 6962-6973.	5.5	37

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19	Early ERP components to emotional facial expressions in young adult victims of childhood maltreatment. Psychiatry Research, 2019, 275, 120-128.	1.7	15
20	The interaction between positive schizotypy and high sensitivity C-reactive protein on response inhibition in female individuals. Psychiatry Research, 2019, 274, 365-371.	1.7	5
21	Prediction of room-temperature half-metallicity in layered halide double perovskites. Npj Computational Materials, 2019, 5, .	3.5	19
22	Unique ion diffusion properties in lead-free halide double perovskites: A first-principles study. Journal of Power Sources, 2019, 412, 689-694.	4.0	12
23	Atomic-Approach to Predict the Energetically Favored Composition Region and to Characterize the Short-, Medium-, and Extended-Range Structures of the Ti-Nb-Al Ternary Metallic Glasses. Materials, 2019, 12, 432.	1.3	1
24	Cation Conformational Changes of 1-Butyl-3-methylimidazolium Halides at High Pressures. Journal of Physical Chemistry C, 2018, 122, 9320-9331.	1.5	2
25	Prediction of Novel pâ€Type Transparent Conductors in Layered Double Perovskites: A Firstâ€Principles Study. Advanced Functional Materials, 2018, 28, 1800332.	7.8	49
26	First-Principle Study of Li-Ion Storage of Functionalized Ti₂C Monolayer with Vacancies. ACS Applied Materials & Interfaces, 2018, 10, 6369-6377.	4.0	89
27	Design of nâ€Type Transparent Conducting Oxides: The Case of Transition Metal Doping in In₂O₃. Advanced Electronic Materials, 2018, 4, 1700553.	2.6	58
28	Fundamental Link between Î² Relaxation, Excess Wings, and Cage-Breaking in Metallic Glasses. Journal of Physical Chemistry Letters, 2018, 9, 5877-5883.	2.1	44
29	Ultrasmall nanoparticles inducing order-to-disorder transition. Physical Review B, 2018, 98, .	1.1	4
30	Common mechanism for controlling polymorph selection during crystallization in supercooled metallic liquids. Acta Materialia, 2018, 161, 367-373.	3.8	19
31	Atomistic simulation study of favored compositions of Ni-Nb-Al metallic glasses. Science China Technological Sciences, 2018, 61, 1829-1838.	2.0	6
32	The prevalence of psychiatric disorders among students aged 6~â€‰16Âyears old in central Hunan, China. BMC Psychiatry, 2018, 18, 243.	1.1	27
33	Atomistic Simulations to Predict Favored Glass-Formation Composition and Ion-Beam-Mixing of Nano-Multiple-Metal-Layers to Produce Ternary Amorphous Films. Metals, 2018, 8, 129.	1.0	2
34	Estimated prevalence and associated risk factors of attention deficit hyperactivity disorder (ADHD) among medical college students in a Chinese population. Journal of Affective Disorders, 2018, 241, 291-296.	2.0	15
35	First-Principles Study of the Charge Transport Mechanisms in Lithium Superoxide. Chemistry of Materials, 2017, 29, 2202-2210.	3.2	30
36	The role of negatively charged oxygen vacancies upon Î²-MnO2 conductivity. Acta Materialia, 2017, 131, 88-97.	3.8	13

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37	Associations between suicidal behavior and childhood abuse and neglect: A meta-analysis. Journal of Affective Disorders, 2017, 220, 147-155.	2.0	100
38	Intrinsic Defect Physics in Indium-based Lead-free Halide Double Perovskites. Journal of Physical Chemistry Letters, 2017, 8, 4391-4396.	2.1	71
39	First-Principles Analysis of Li Intercalation in VO₂(B). Chemistry of Materials, 2017, 29, 10075-10087.	3.2	28
40	Abnormalities of localized connectivity in schizophrenia patients and their unaffected relatives: a meta-analysis of resting-state functional magnetic resonance imaging studies. Neuropsychiatric Disease and Treatment, 2017, Volume 13, 467-475.	1.0	36
41	Perceived parental rejection mediates the effects of previous maltreatment on emotional and behavioural outcomes in Chinese adolescents whereas mental illness has no moderating effect. South African Journal of Psychiatry, 2017, 23, 1073.	0.2	2
42	First principles study of nanostructured TiS2 electrodes for Na and Mg ion storage. Journal of Power Sources, 2016, 320, 322-331.	4.0	46
43	Self-healing properties of nanocrystalline materials: a first-principles analysis of the role of grain boundaries. Physical Chemistry Chemical Physics, 2016, 18, 17930-17940.	1.3	21
44	Atomistic approach to design favored compositions for the ternary Alâ€“Mgâ€“Ca metallic glass formation. RSC Advances, 2015, 5, 93623-93630.	1.7	4
45	Atomistic study of chemical effect on local structure in Mg-based metallic glasses. RSC Advances, 2015, 5, 46861-46868.	1.7	0
46	Composition-Dependent Structural and Electronic Properties of Mg95â€“xZnxCa5Metallic Glasses: An Ab Initio Molecular Dynamics Study. Journal of Physical Chemistry B, 2015, 119, 3608-3618.	1.2	9
47	Migrations of Pentagonâ€“Heptagon Defects in Hexagonal Boron Nitride Monolayer: The First-Principles Study. Journal of Physical Chemistry A, 2015, 119, 3621-3627.	1.1	9
48	Phase stability and mechanical properties of sigma phase in Coâ€“Mo system by first principles calculations. Computational Materials Science, 2015, 98, 424-429.	1.4	10
49	Atomic approach to the optimized compositions of Niâ€“Nbâ€“Ti glassy alloys with large glass-forming ability. RSC Advances, 2015, 5, 3054-3062.	1.7	12
50	Predicting Composition Dependence of Glass Forming Ability in Ternary Al-Cu-Y System by Thermodynamic Calculation. Metals, 2014, 4, 519-529.	1.0	7
51	First Principles Study of Structural Stability and Magnetic Property of Non-equilibrium Coâ€“Mo Alloys. Acta Metallurgica Sinica (English Letters), 2014, 27, 1057-1062.	1.5	2
52	First principle predictions of anomalous yield strength in L1₂materials. Materials Research Innovations, 2014, 18, S4-1021-S4-1025.	1.0	5
53	Interatomic potential to predict the glass-forming ability of Niâ€“Nbâ€“Mo ternary alloys. Journal of Materials Science, 2014, 49, 7263-7272.	1.7	4
54	Structural skeleton of preferentially interpenetrated clusters and correlation with shear localization in Mgâ€“Cuâ€“Ni ternary metallic glasses. Physical Chemistry Chemical Physics, 2014, 16, 19590.	1.3	19

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55	Favored Composition Design and Atomic Structure Characterization for Ternary Alâ€“Cuâ€“Y Metallic Glasses via Proposed Interatomic Potential. Journal of Physical Chemistry B, 2014, 118, 4442-4449.	1.2	16
56	In situ high resolution transmission electron microscopy investigation of deformation mechanism in sub-10-nm Au crystals. Materials Science and Technology, 2014, 30, 774-781.	0.8	6
57	Atomic modeling to design favored compositions for the ternary Niâ€“Nbâ€“Zr metallic glass formation. Acta Materialia, 2014, 76, 482-492.	3.8	11
58	Different atomic structures observed from ternary Ni-Nb-Ta metallic glasses obtained by ion beam mixing. Science China Technological Sciences, 2013, 56, 1842-1846.	2.0	1
59	Calculation of driving force and local order to predict the favored and optimized compositions for Mg-Cu-Ni metallic glass formation. Journal of Applied Physics, 2013, 114, 153503.	1.1	3
60	Metallic glass formation in the ternary Ni-Nb-Mo system by ion beam mixing. Science China Technological Sciences, 2012, 55, 2206-2211.	2.0	3
61	Transmission electron microscopy observation of a deformation twin in TWIP steel by anex situtensile test. Philosophical Magazine, 2011, 91, 4033-4044.	0.7	9
62	Phase orientation, interface structure, and properties of aged Cu-6 wt.% Ag. Journal of Materials Science, 2008, 43, 2006-2011.	1.7	21
63	Relationships between mechanical strength and electrical conductivity for Cuâ€“Ag filamentary microcomposites. Applied Physics A: Materials Science and Processing, 2007, 86, 529-532.	1.1	13
64	Predicting yield-stress anomalies in L12 alloys: Ni3Geâ€“Fe3Ge pseudo-binaries. Acta Materialia, 2005, 53, 3601-3612.	3.8	28
65	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
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	Comparative study of nonequilibrium phase of A3B and AB3 types in the Niâ€“Mo system by first principles and thermodynamic calculations. Journal of Materials Research, 2002, 17, 2720-2726.	1.2	2