Shijun Zhao

List of Publications by Year
in descending order

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95 papers	4,759 citations	94433 37 h-index	98798 67 g-index
95 all docs	95 docs citations	95 times ranked	4241 citing authors

#	Article	IF	Citations
1	The potential application of phosphorene as an anode material in Li-ion batteries. Journal of Materials Chemistry A, 2014, 2, 19046-19052.	10.3	339
2	Stacking fault energies of face-centered cubic concentrated solid solution alloys. Acta Materialia, 2017, 134, 334-345.	7.9	330
3	Gas adsorption on MoS2 monolayer from first-principles calculations. Chemical Physics Letters, 2014, 595-596, 35-42.	2.6	328
4	Local Structure and Short-Range Order in a NiCoCr Solid Solution Alloy. Physical Review Letters, 2017, 118, 205501.	7.8	283
5	Activating lattice oxygen in NiFe-based (oxy)hydroxide for water electrolysis. Nature Communications, 2022, 13, 2191.	12.8	179
6	Atomic-level heterogeneity and defect dynamics in concentrated solid-solution alloys. Current Opinion in Solid State and Materials Science, 2017, 21, 221-237.	11.5	155
7	Defect energetics of concentrated solid-solution alloys from ab initio calculations: Ni_{0.5}Co_{0.5}, Ni_{0.5}Fe_{0.5}, Ni_{0.8}Fe_{0.2}and Ni_{0.8}Cr_{0.2}. Physical Chemistry Chemical Physics, 2016, 18, 24043-24056.	2.8	148
8	Manipulation of electronic and magnetic properties of M2C (M = Hf, Nb, Sc, Ta, Ti, V, Zr) monolayer by applying mechanical strains. Applied Physics Letters, 2014, 104, .	3.3	139
9	Preferential diffusion in concentrated solid solution alloys: NiFe, NiCo and NiCoCr. Acta Materialia, 2017, 128, 391-399.	7.9	124
10	Mechanical properties of hybrid graphene and hexagonal boron nitride sheets as revealed by molecular dynamic simulations. Journal Physics D: Applied Physics, 2013, 46, 135303.	2.8	116
11	Influence of chemical disorder on energy dissipation and defect evolution in advanced alloys. Journal of Materials Research, 2016, 31, 2363-2375.	2.6	110
12	High adsorption capacity of heavy metals on two-dimensional MXenes: an ab initio study with molecular dynamics simulation. Physical Chemistry Chemical Physics, 2016, 18, 228-233.	2.8	109
13	Severe local lattice distortion in Zr- and/or Hf-containing refractory multi-principal element alloys. Acta Materialia, 2020, 183, 172-181.	7.9	108
14	Ion selection of charge-modified large nanopores in a graphene sheet. Journal of Chemical Physics, 2013, 139, 114702.	3.0	95
15	Role of Strain and Concentration on the Li Adsorption and Diffusion Properties on Ti₂C Layer. Journal of Physical Chemistry C, 2014, 118, 14983-14990.	3.1	88
16	Local-environment dependence of stacking fault energies in concentrated solid-solution alloys. Npj Computational Materials, 2019, 5, .	8.7	80
17	Defect properties in a VTaCrW equiatomic high entropy alloy (HEA) with the body centered cubic (bcc) structure. Journal of Materials Science and Technology, 2020, 44, 133-139.	10.7	77
18	Effect of d electrons on defect properties in equiatomic NiCoCr and NiCoFeCr concentrated solid solution alloys. Physical Review Materials, 2018, 2, .	2.4	72

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19	Ab initio study of irradiation tolerance for different Mn+1AXn phases: Ti3SiC2 and Ti3AlC2. Journal of Applied Physics, 2014, 115, .	2.5	69
20	Evolution of local lattice distortion under irradiation in medium- and high-entropy alloys. Materialia, 2018, 2, 73-81.	2.7	67
21	Mechanism of the Defect Formation in Supported Graphene by Energetic Heavy Ion Irradiation: the Substrate Effect. Scientific Reports, 2015, 5, 9935.	3.3	66
22	MXene nanoribbons. Journal of Materials Chemistry C, 2015, 3, 879-888.	5.5	65
23	Pressure-induced fcc to hcp phase transition in Ni-based high entropy solid solution alloys. Applied Physics Letters, 2017, 110, .	3.3	62
24	Atomic-scale dynamics of edge dislocations in Ni and concentrated solid solution NiFe alloys. Journal of Alloys and Compounds, 2017, 701, 1003-1008.	5.5	59
25	Fabrication of nanopores in a graphene sheet with heavy ions: A molecular dynamics study. Journal of Applied Physics, 2013, 114, .	2.5	55
26	Facile, cost-effective plasma synthesis of self-supportive FeS_x on Fe foam for efficient electrochemical reduction of N₂ under ambient conditions. Journal of Materials Chemistry A, 2019, 7, 19977-19983.	10.3	50
27	Lattice distortion in highâ€entropy carbide ceramics from firstâ€principles calculations. Journal of the American Ceramic Society, 2021, 104, 1874-1886.	3.8	50
28	Effect of SiO₂substrate on the irradiation-assisted manipulation of supported graphene: a molecular dynamics study. Nanotechnology, 2012, 23, 285703.	2.6	47
29	Irradiation responses and defect behavior of single-phase concentrated solid solution alloys. Journal of Materials Research, 2018, 33, 3077-3091.	2.6	47
30	Suppression of vacancy cluster growth in concentrated solid solution alloys. Acta Materialia, 2017, 125, 231-237.	7.9	45
31	A comparison study of local lattice distortion in Ni80Pd20 binary alloy and FeCoNiCrPd high-entropy alloy. Scripta Materialia, 2018, 156, 14-18.	5.2	45
32	Drilling Nanopores in Graphene with Clusters: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2012, 116, 11776-11782.	3.1	44
33	Helium irradiated cavity formation and defect energetics in Ni-based binary single-phase concentrated solid solution alloys. Acta Materialia, 2019, 164, 283-292.	7.9	44
34	Strengthening in Al-, Mo- or Ti-doped CoCrFeNi high entropy alloys: A parallel comparison. Journal of Materials Science and Technology, 2021, 94, 264-274.	10.7	44
35	Modification of graphene supported on SiO2 substrate with swift heavy ions from atomistic simulation point. Carbon, 2015, 93, 169-179.	10.3	42
36	Diffusion controlled helium bubble formation resistance of FeCoNiCr high-entropy alloy in the half-melting temperature regime. Journal of Nuclear Materials, 2019, 526, 151747.	2.7	40

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37	Delayed damage accumulation by athermal suppression of defect production in concentrated solid solution alloys. Materials Research Letters, 2018, 6, 136-141.	8.7	39
38	Phase, microstructure and related mechanical properties of a series of (NbTaZr)C-Based high entropy ceramics. Ceramics International, 2021, 47, 14341-14347.	4.8	38
39	Frenkel defect recombination in Ni and Niâ€'containing concentrated solidâ€'solution alloys. Acta Materialia, 2019, 173, 184-194.	7.9	37
40	Design high-entropy carbide ceramics from machine learning. Npj Computational Materials, 2022, 8, .	8.7	37
41	Defect accumulation and evolution in refractory multi-principal element alloys. Acta Materialia, 2021, 219, 117233.	7.9	36
42	Strain-tunable electronic properties and lithium storage of 2D transition metal carbide (MXene) Ti₂CO₂ as a flexible electrode. Journal of Materials Chemistry A, 2020, 8, 760-769.	10.3	35
43	Unique Challenges for Modeling Defect Dynamics in Concentrated Solid-Solution Alloys. Jom, 2017, 69, 2084-2091.	1.9	33
44	Diffusion of point defects in ordered and disordered Niâ€"Fe alloys. Journal of Alloys and Compounds, 2019, 805, 1175-1183.	5.5	33
45	Microalloyed medium-entropy alloy (MEA) composite nanolattices with ultrahigh toughness and cyclability. Materials Today, 2021, 42, 10-16.	14.2	32
46	High-entropy carbide ceramics: a perspective review. Tungsten, 2021, 3, 131-142.	4.8	31
47	Effect of silicon addition on the microstructures, mechanical properties and helium irradiation resistance of NiCoCr-based medium-entropy alloys. Journal of Alloys and Compounds, 2020, 844, 156162.	5.5	30
48	Link between<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>K</mml:mi></mml:math>absorption edges and thermodynamic properties of warm dense plasmas established by an improved first-principles method. Physical Review B, 2016, 93, .	3.2	28
49	Elemental partitions and deformation mechanisms of L12-type multicomponent intermetallics. Acta Materialia, 2021, 219, 117238.	7.9	28
50	Comparison of electronic energy loss in graphene and BN sheet by means of time-dependent density functional theory. Journal of Physics Condensed Matter, 2015, 27, 025401.	1.8	27
51	Tuning the band gap of bilayer graphene by ion implantation: Insight from computational studies. Physical Review B, 2012, 86, .	3.2	26
52	Effects of local elemental ordering on defect-grain boundary interactions in high-entropy alloys. Journal of Alloys and Compounds, 2021, 887, 161314.	5.5	22
53	First-principles study of He behavior in a NiCoFeCr concentrated solidâ€"solution alloy. Materials Research Letters, 2019, 7, 188-193.	8.7	21
54	Defect-Mediated Adsorption of Metal Ions for Constructing Ni Hydroxide/MoS₂ Heterostructures as High-Performance Water-Splitting Electrocatalysts. ACS Applied Energy Materials, 2020, 3, 7039-7047.	5.1	20

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55	Application of machine learning in understanding the irradiation damage mechanism of high-entropy materials. Journal of Nuclear Materials, 2022, 559, 153462.	2.7	18
56	First-principles investigation of the intrinsic defects in Ti3SiC2. Journal of Physics and Chemistry of Solids, 2014, 75, 384-390.	4.0	17
57	Revealing the crucial role of rough energy landscape on self-diffusion in high-entropy alloys based on machine learning and kinetic Monte Carlo. Acta Materialia, 2022, 234, 118051.	7.9	17
58	Role of chemical disorder and local ordering on defect evolution in high-entropy alloys. Physical Review Materials, 2021, 5, .	2.4	16
59	Chemical short-range ordering regulated dislocation cross slip in high-entropy alloys. Journal of Alloys and Compounds, 2022, 911, 165144.	5.5	16
60	Stability of vacancy-type defect clusters in Ni based on first-principles and molecular dynamics simulations. Scripta Materialia, 2018, 145, 71-75.	5.2	15
61	Fluctuations in stacking fault energies improve irradiation tolerance of concentrated solid-solution alloys. Journal of Nuclear Materials, 2020, 530, 151886.	2.7	15
62	On the role of heterogeneity in concentrated solid-solution alloys in enhancing their irradiation resistance. Journal of Materials Research, 2020, 35, 1103-1112.	2.6	15
63	Effects of minor alloying addition on He bubble formation in the irradiated FeCoNiCr-based high-entropy alloys. Journal of Nuclear Materials, 2020, 542, 152458.	2.7	15
64	Local Ordering Tendency in Body-Centered Cubic (BCC) Multi-Principal Element Alloys. Journal of Phase Equilibria and Diffusion, 2021, 42, 578-591.	1.4	15
65	Toughening (NbTaZrW)C highâ€entropy carbide ceramic through Mo doping. Journal of the American Ceramic Society, 2022, 105, 5395-5407.	3.8	15
66	He-enhanced heterogeneity of radiation-induced segregation in FeNiCoCr high-entropy alloy. Journal of Materials Science and Technology, 2022, 101, 226-233.	10.7	14
67	Alloying effects on lowâ€'energy recoil events in concentrated solidâ€'solution alloys. Journal of Nuclear Materials, 2020, 529, 151941.	2.7	12
68	The stability of Î³â€² precipitates in a multi-component FeCoNiCrTi0.2 alloy under elevated-temperature irradiation. Journal of Nuclear Materials, 2020, 540, 152364.	2.7	12
69	Structural and chemical disorder enhance point defect diffusion and atomic transport in Ni3Al-based Î³â€² phase. Acta Materialia, 2021, 207, 116704.	7.9	11
70	Local structure of NiPd solid solution alloys and its response to ion irradiation. Journal of Alloys and Compounds, 2018, 755, 242-250.	5.5	10
71	Self-irradiation of thin SiC nanowires with low-energy ions: a molecular dynamics study. Journal Physics D: Applied Physics, 2012, 45, 135403.	2.8	9
72	H+ (D+, T+)â€"beryllium collisions studied using time-dependent density functional theory. Physics Letters, Section A: General, Atomic and Solid State Physics, 2015, 379, 319-326.	2.1	9

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73	Engineering defect energy landscape of CoCrFeNi high-entropy alloys by the introduction of additional dopants. Journal of Nuclear Materials, 2022, 561, 153573.	2.7	9
74	Influence of high pressure on the threshold displacement energies in silicon carbide: A Carâ€“Parrinello molecular dynamics approach. Nuclear Instruments & Methods in Physics Research B, 2012, 286, 119-123.	1.4	8
75	First-principles calculation of principal Hugoniot and K-shell X-ray absorption spectra for warm dense KCl. Physics of Plasmas, 2015, 22, 062707.	1.9	8
76	First-Principles Investigation to Ionization of Argon Under Conditions Close to Typical Sonoluminescence Experiments. Scientific Reports, 2016, 6, 20623.	3.3	8
77	High Entropy Alloys: Irradiation. , 2020, , .		8
78	Effects of temperature on helium cavity evolution in single-phase concentrated solid-solution alloys. Journal of Nuclear Materials, 2021, 557, 153261.	2.7	8
79	Defect energetics and stacking fault formation in high-entropy carbide ceramics. Journal of the European Ceramic Society, 2022, 42, 5290-5302.	5.7	8
80	Chemical bonding assisted damage production in single-walled carbon nanotubes induced by low-energy ions. Applied Physics A: Materials Science and Processing, 2012, 108, 313-320.	2.3	7
81	Ab Initio Study of Electronic Excitation Effects on SrTiO₃. Journal of Physical Chemistry C, 2017, 121, 26622-26628.	3.1	7
82	Atomistic insight into the effects of order, disorder and their interface on defect evolution. Journal of Alloys and Compounds, 2021, 859, 157770.	5.5	7
83	Study on the effect of pressure on the properties of intrinsic point defects in monoclinic zirconia: Ab initio calculations. Journal of Applied Physics, 2012, 111, .	2.5	6
84	Enhanced recombination suppresses the void swelling in bcc multi-component alloys. Materialia, 2021, 20, 101234.	2.7	6
85	Softening Al13Fe4 intermetallic compound through Fe-site multi-principal-element doping. Scripta Materialia, 2022, 218, 114811.	5.2	6
86	Instability-free ion acceleration by two laser pulses. European Physical Journal: Special Topics, 2014, 223, 1031-1035.	2.6	5
87	Atomistic simulation of defect-dislocation interactions in concentrated solid-solution alloys. Physical Review Materials, 2019, 3, .	2.4	5
88	Manipulating the Resistive Switching in Epitaxial SrCoO_{2.5} Thin-Film-Based Memristors by Strain Engineering. ACS Applied Electronic Materials, 2022, 4, 2729-2738.	4.3	5
89	X-ray absorption investigation of local structural disorder in Ni1-xFex (xâ€‰=â€‰0.10, 0.20, 0.35, and 0.50) alloys. Journal of Applied Physics, 2017, 121, 165105.	2.5	4
90	Temperature-dependent helium induced microstructural evolution in equiatomic NiCo and NiFe concentrated solid solution alloys. Journal of Nuclear Materials, 2021, 545, 152715.	2.7	4

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91	Influence of temperature and alloying elements on the threshold displacement energies in concentrated Niâ€“Feâ€“Cr alloys*. Chinese Physics B, 2021, 30, 056111.	1.4	4
92	Defect evolution mechanism in U3Si2 from molecular dynamics simulations. Journal of Nuclear Materials, 2020, 537, 152238.	2.7	4
93	A Model for Dose Dependence of the Void Swelling in Electron-Irradiated Alloys. Metals, 2022, 12, 244.	2.3	3
94	Additivity of kinetic and potential energy contributions in modification of graphene supported onSiO2. Nuclear Instruments & Methods in Physics Research B, 2017, 397, 62-66.	1.4	2
95	Effects of local chemical ordering on defect evolution in NiFe concentrated solid solution alloy. Journal of Nuclear Materials, 2022, 568, 153877.	2.7	2