Shijun Zhao

List of Publications by Citations

89 papers	2,899 citations	29 h-index	52 g-index
95 ext. papers	3,799 ext. citations	5.3 avg, IF	6.11 L-index

#	Paper	IF	Citations
89	The potential application of phosphorene as an anode material in Li-ion batteries. *Journal of Materials Chemistry A*, **2014**, 2, 19046-19052	13	254
88	Gas adsorption on MoS2 monolayer from first-principles calculations. *Chemical Physics Letters*, **2014** , 595-596, 35-42	2.5	248
87	Stacking fault energies of face-centered cubic concentrated solid solution alloys. *Acta Materialia*, **2017**, 134, 334-345	8.4	206
86	Local Structure and Short-Range Order in a NiCoCr Solid Solution Alloy. *Physical Review Letters*, **2017**, 118, 205501	7.4	156
85	Atomic-level heterogeneity and defect dynamics in concentrated solid-solution alloys. *Current Opinion in Solid State and Materials Science*, **2017**, 21, 221-237	12	110
84	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, 133106	3.4	109
83	Defect energetics of concentrated solid-solution alloys from ab initio calculations: Ni0.5Co0.5, Ni0.5Fe0.5, Ni0.8Fe0.2 and Ni0.8Cr0.2. *Physical Chemistry Chemical Physics*, **2016**, 18, 24043-56	3.6	99
82	Mechanical properties of hybrid graphene and hexagonal boron nitride sheets as revealed by molecular dynamic simulations. *Journal Physics D: Applied Physics*, **2013**, 46, 135303	3	92
81	Preferential diffusion in concentrated solid solution alloys: NiFe, NiCo and NiCoCr. *Acta Materialia*, **2017**, 128, 391-399	8.4	88
80	Influence of chemical disorder on energy dissipation and defect evolution in advanced alloys. *Journal of Materials Research*, **2016**, 31, 2363-2375	2.5	78
79	High adsorption capacity of heavy metals on two-dimensional MXenes: an ab initio study with molecular dynamics simulation. *Physical Chemistry Chemical Physics*, **2016**, 18, 228-33	3.6	75
78	Ion selection of charge-modified large nanopores in a graphene sheet. *Journal of Chemical Physics*, **2013**, 139, 114702	3.9	75
77	Role of Strain and Concentration on the Li Adsorption and Diffusion Properties on Ti2C Layer. *Journal of Physical Chemistry C*, **2014**, 118, 14983-14990	3.8	72
76	Ab initio study of irradiation tolerance for different Mn+1AXn phases: Ti3SiC2 and Ti3AlC2. *Journal of Applied Physics*, **2014**, 115, 023503	2.5	63
75	Mechanism of the defect formation in supported graphene by energetic heavy ion irradiation: the substrate effect. *Scientific Reports*, **2015**, 5, 9935	4.9	54
74	Severe local lattice distortion in Zr- and/or Hf-containing refractory multi-principal element alloys. *Acta Materialia*, **2020**, 183, 172-181	8.4	53
73	MXene nanoribbons. *Journal of Materials Chemistry C*, **2015**, 3, 879-888	7.1	51

72	Pressure-induced fcc to hcp phase transition in Ni-based high entropy solid solution alloys. *Applied Physics Letters*, **2017**, 110, 011902	3.4	50
71	Evolution of local lattice distortion under irradiation in medium- and high-entropy alloys. *Materialia*, **2018**, 2, 73-81	3.2	46
70	Local-environment dependence of stacking fault energies in concentrated solid-solution alloys. *Npj Computational Materials*, **2019**, 5,	10.9	45
69	Fabrication of nanopores in a graphene sheet with heavy ions: A molecular dynamics study. *Journal of Applied Physics*, **2013**, 114, 234304	2.5	44
68	Effect of SiO2 substrate on the irradiation-assisted manipulation of supported graphene: a molecular dynamics study. *Nanotechnology*, **2012**, 23, 285703	3.4	42
67	Effect of d electrons on defect properties in equiatomic NiCoCr and NiCoFeCr concentrated solid solution alloys. *Physical Review Materials*, **2018**, 2,	3.2	42
66	Drilling Nanopores in Graphene with Clusters: A Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2012**, 116, 11776-11782	3.8	38
65	Atomic-scale dynamics of edge dislocations in Ni and concentrated solid solution NiFe alloys. *Journal of Alloys and Compounds*, **2017**, 701, 1003-1008	5.7	37
64	Suppression of vacancy cluster growth in concentrated solid solution alloys. *Acta Materialia*, **2017**, 125, 231-237	8.4	35
63	Delayed damage accumulation by athermal suppression of defect production in concentrated solid solution alloys. *Materials Research Letters*, **2018**, 6, 136-141	7.4	31
62	Modification of graphene supported on SiO2 substrate with swift heavy ions from atomistic simulation point. *Carbon*, **2015**, 93, 169-179	10.4	30
61	Helium irradiated cavity formation and defect energetics in Ni-based binary single-phase concentrated solid solution alloys. *Acta Materialia*, **2019**, 164, 283-292	8.4	30
60	A comparison study of local lattice distortion in Ni80Pd20 binary alloy and FeCoNiCrPd high-entropy alloy. *Scripta Materialia*, **2018**, 156, 14-18	5.6	28
59	Facile, cost-effective plasma synthesis of self-supportive FeSx on Fe foam for efficient electrochemical reduction of N2 under ambient conditions. *Journal of Materials Chemistry A*, **2019**, 7, 19977-19983	13	28
58	Irradiation responses and defect behavior of single-phase concentrated solid solution alloys. *Journal of Materials Research*, **2018**, 33, 3077-3091	2.5	28
57	Unique Challenges for Modeling Defect Dynamics in Concentrated Solid-Solution Alloys. *Jom*, **2017**, 69, 2084-2091	2.1	27
56	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	9.1	25
55	Tuning the band gap of bilayer graphene by ion implantation: Insight from computational studies. *Physical Review B*, **2012**, 86,	3.3	24

54	Frenkel defect recombination in Ni and Ni-containing concentrated solid-solution alloys. *Acta Materialia*, **2019**, 173, 184-194	8.4	23
53	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	23
52	Link between K absorption edges and thermodynamic properties of warm dense plasmas established by an improved first-principles method. *Physical Review B*, **2016**, 93,	3.3	22
51	Diffusion controlled helium bubble formation resistance of FeCoNiCr high-entropy alloy in the half-melting temperature regime. *Journal of Nuclear Materials*, **2019**, 526, 151747	3.3	19
50	Diffusion of point defects in ordered and disordered NiFe alloys. *Journal of Alloys and Compounds*, **2019**, 805, 1175-1183	5.7	18
49	Activating lattice oxygen in NiFe-based (oxy)hydroxide for water electrolysis.. *Nature Communications*, **2022**, 13, 2191	17.4	16
48	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	13	15
47	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	6.1	14
46	Strengthening in Al-, Mo- or Ti-doped CoCrFeNi high entropy alloys: A parallel comparison. *Journal of Materials Science and Technology*, **2021**, 94, 264-274	9.1	13
45	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	5.7	12
44	First-principles investigation of the intrinsic defects in Ti3SiC2. *Journal of Physics and Chemistry of Solids*, **2014**, 75, 384-390	3.9	12
43	First-principles study of He behavior in a NiCoFeCr concentrated solid solution alloy. *Materials Research Letters*, **2019**, 7, 188-193	7.4	11
42	Phase, microstructure and related mechanical properties of a series of (NbTaZr)C-Based high entropy ceramics. *Ceramics International*, **2021**, 47, 14341-14347	5.1	11
41	Lattice distortion in high-entropy carbide ceramics from first-principles calculations. *Journal of the American Ceramic Society*, **2021**, 104, 1874-1886	3.8	11
40	Microalloyed medium-entropy alloy (MEA) composite nanolattices with ultrahigh toughness and cyclability. *Materials Today*, **2021**, 42, 10-16	21.8	10
39	Fluctuations in stacking fault energies improve irradiation tolerance of concentrated solid-solution alloys. *Journal of Nuclear Materials*, **2020**, 530, 151886	3.3	9
38	On the role of heterogeneity in concentrated solid-solution alloys in enhancing their irradiation resistance. *Journal of Materials Research*, **2020**, 35, 1103-1112	2.5	9
37	Self-irradiation of thin SiC nanowires with low-energy ions: a molecular dynamics study. *Journal Physics D: Applied Physics*, **2012**, 45, 135403	3	8

36	First-Principles Investigation to Ionization of Argon Under Conditions Close to Typical Sonoluminescence Experiments. *Scientific Reports*, **2016**, 6, 20623	4.9	8
35	H+ (D+, T+)Beryllium collisions studied using time-dependent density functional theory. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2015**, 379, 319-326	2.3	7
34	First-principles calculation of principal Hugoniot and K-shell X-ray absorption spectra for warm dense KCl. *Physics of Plasmas*, **2015**, 22, 062707	2.1	7
33	Influence of high pressure on the threshold displacement energies in silicon carbide: A Car-Parrinello molecular dynamics approach. *Nuclear Instruments & Methods in Physics Research B*, **2012**, 286, 119-123	1.2	7
32	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	2.6	7
31	High-entropy carbide ceramics: a perspective review. *Tungsten*, **2021**, 3, 131-142	4.6	7
30	Local structure of NiPd solid solution alloys and its response to ion irradiation. *Journal of Alloys and Compounds*, **2018**, 755, 242-250	5.7	6
29	Stability of vacancy-type defect clusters in Ni based on first-principles and molecular dynamics simulations. *Scripta Materialia*, **2018**, 145, 71-75	5.6	6
28	Effects of minor alloying addition on He bubble formation in the irradiated FeCoNiCr-based high-entropy alloys. *Journal of Nuclear Materials*, **2020**, 542, 152458	3.3	6
27	Structural and chemical disorder enhance point defect diffusion and atomic transport in Ni3Al-based γ′ phase. *Acta Materialia*, **2021**, 207, 116704	8.4	6
26	High Entropy Alloys: Irradiation **2020**,		5
25	Alloying effects on low-energy recoil events in concentrated solid-solution alloys. *Journal of Nuclear Materials*, **2020**, 529, 151941	3.3	5
24	The stability of γ′ precipitates in a multi-component FeCoNiCrTi0.2 alloy under elevated-temperature irradiation. *Journal of Nuclear Materials*, **2020**, 540, 152364	3.3	5
23	Instability-free ion acceleration by two laser pulses. *European Physical Journal: Special Topics*, **2014**, 223, 1031-1035	2.3	4
22	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, 043514	2.5	4
21	Atomistic simulation of defect-dislocation interactions in concentrated solid-solution alloys. *Physical Review Materials*, **2019**, 3,	3.2	4
20	Defect accumulation and evolution in refractory multi-principal element alloys. *Acta Materialia*, **2021**, 219, 117233	8.4	4
19	Effects of local elemental ordering on defect-grain boundary interactions in high-entropy alloys. *Journal of Alloys and Compounds*, **2021**, 887, 161314	5.7	4

18	Ab Initio Study of Electronic Excitation Effects on SrTiO3. *Journal of Physical Chemistry C*, **2017**, 121, 26628-26638	3.3	3
17	Local Ordering Tendency in Body-Centered Cubic (BCC) Multi-Principal Element Alloys. *Journal of Phase Equilibria and Diffusion*,1	1	3
16	X-ray absorption investigation of local structural disorder in Ni1-xFex (x = 0.10, 0.20, 0.35, and 0.50) alloys. *Journal of Applied Physics*, **2017**, 121, 165105	2.5	2
15	Application of machine learning in understanding the irradiation damage mechanism of high-entropy materials. *Journal of Nuclear Materials*, **2022**, 559, 153462	3.3	2
14	Elemental partitions and deformation mechanisms of L12-type multicomponent intermetallics. *Acta Materialia*, **2021**, 219, 117238	8.4	2
13	He-enhanced heterogeneity of radiation-induced segregation in FeNiCoCr high-entropy alloy. *Journal of Materials Science and Technology*, **2022**, 101, 226-233	9.1	2
12	Chemical short-range ordering regulated dislocation cross slip in high-entropy alloys. *Journal of Alloys and Compounds*, **2022**, 911, 165144	5.7	2
11	Additivity of kinetic and potential energy contributions in modification of graphene supported onSiO2. *Nuclear Instruments & Methods in Physics Research B*, **2017**, 397, 62-66	1.2	1
10	Engineering defect energy landscape of CoCrFeNi high-entropy alloys by the introduction of additional dopants. *Journal of Nuclear Materials*, **2022**, 561, 153573	3.3	1
9	Defect evolution mechanism in U3Si2 from molecular dynamics simulations. *Journal of Nuclear Materials*, **2020**, 537, 152238	3.3	1
8	Influence of temperature and alloying elements on the threshold displacement energies in concentrated NiFeCr alloys*. *Chinese Physics B*, **2021**, 30, 056111	1.2	1
7	Atomistic insight into the effects of order, disorder and their interface on defect evolution. *Journal of Alloys and Compounds*, **2021**, 859, 157770	5.7	1
6	Enhanced recombination suppresses the void swelling in bcc multi-component alloys. *Materialia*, **2021**, 20, 101234	3.2	1
5	Effects of temperature on helium cavity evolution in single-phase concentrated solid-solution alloys. *Journal of Nuclear Materials*, **2021**, 557, 153261	3.3	1
4	A Model for Dose Dependence of the Void Swelling in Electron-Irradiated Alloys. *Metals*, **2022**, 12, 244	2.3	0
3	Temperature-dependent helium induced microstructural evolution in equiatomic NiCo and NiFe concentrated solid solution alloys. *Journal of Nuclear Materials*, **2021**, 545, 152715	3.3	0
2	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	8.4	0
1	Softening Al13Fe4 intermetallic compound through Fe-site multi-principal-element doping. *Scripta Materialia*, **2022**, 218, 114811	5.6	0