Chong-Yu Wang

List of Publications by Citations

77 papers	1,259 citations	21 h-index	32 g-index
81 ext. papers	1,464 ext. citations	3.1 avg, IF	4.85 L-index

#	Paper	IF	Citations
77	Energetics and local spin magnetic moment of single 3,4d impurities encapsulated in an icosahedral Au12 cage. *Physical Review B*, **2004**, 70,	3.3	68
76	The effect of alloying elements on the dislocation climbing velocity in Ni: A first-principles study. *Acta Materialia*, **2009**, 57, 5914-5920	8.4	65
75	A comparison of the ideal strength between L12Co3(Al,W) and Ni3Al under tension and shear from first-principles calculations. *Applied Physics Letters*, **2009**, 94, 261909	3.4	62
74	Misfit dislocation networks in the □ phase interface of a Ni-based single-crystal superalloy: Molecular dynamics simulations. *Physical Review B*, **2005**, 72,	3.3	57
73	The effects of alloying elements on generalized stacking fault energies, strength and ductility of □-Ni3Al. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2012**, 539, 38-41	5.3	47
72	Phase Diagram of Ising Nano-Particles with Cubic Structures. *Physica Status Solidi (B): Basic Research* , **2002**, 232, 254-263	1.3	47
71	Influence of the alloying element Re on the ideal tensile and shear strength of □-Ni3Al. *Scripta Materialia*, **2009**, 61, 197-200	5.6	44
70	Effect of Re in □ phase, □□ phase and □/□□ interface of Ni-based single-crystal superalloys. *Acta Materialia*, **2010**, 58, 2045-2055	8.4	44
69	Energetics and electronic structure of Re and Ta in the □ phase of Ni-based superalloys. *Physical Review B*, **2001**, 65,	3.3	42
68	First-principles study of the stability of the icosahedral Ti13, Ti13□, and Ti13+1 clusters. *Physical Review B*, **2002**, 65,	3.3	39
67	The alloying mechanisms of Re, Ru in the quaternary Ni-based superalloys interface: A first principles calculation. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2008**, 490, 242-249	5.3	35
66	Predicting creep rupture life of Ni-based single crystal superalloys using divide-and-conquer approach based machine learning. *Acta Materialia*, **2020**, 195, 454-467	8.4	35
65	Ni/Ni3Al interface: A density functional theory study. *Applied Surface Science*, **2009**, 255, 3669-3675	6.7	33
64	Motion of misfit dislocation in an Ni/Ni3Al interface: a molecular dynamics simulations study. *Modelling and Simulation in Materials Science and Engineering*, **2009**, 17, 055007	2	33
63	Partitioning and diffusion of transition metal solutes in ternary model Ni-based single crystal superalloys. *Materials and Design*, **2017**, 130, 157-165	8.1	28
62	First-principle investigation of 3d transition metal elements in □-Co3(Al,W). *Journal of Applied Physics*, **2010**, 107, 093705	2.5	28
61	Influence of Re on the propagation of a Ni/Ni3Al interface crack by molecular dynamics simulation. *Modelling and Simulation in Materials Science and Engineering*, **2013**, 21, 045009	2	25

60	Density functional theory study of Ni/Ni3Al interface alloying with Re and Ru. *Surface Science*, **2008**, 602, 2604-2609	1.8	25
59	First-principles study of contact between Ti surface and semiconducting carbon nanotube. *Journal of Applied Physics*, **2007**, 102, 013709	2.5	23
58	Electronic states and doping effect of carbon in the edge-dislocation core of bcc iron. *Physical Review B*, **2004**, 69,	3.3	23
57	First-principles study of point defects in solar cell semiconductor CuI. *Physica B: Condensed Matter*, **2013**, 413, 116-119	2.8	21
56	Effect of interactions between elements on the diffusion of solutes in Ni X Y systems and γ′-coarsening in model Ni-based superalloys. *Scripta Materialia*, **2017**, 138, 100-104	5.6	20
55	Molecular dynamics simulations of influence of Re on lattice trapping and fracture stress of cracks in Ni. *Computational Materials Science*, **2014**, 83, 196-206	3.2	19
54	Influence of alloying elements on the elastic properties of ternary and quaternary nickel-base superalloys. *Philosophical Magazine*, **2009**, 89, 2935-2947	1.6	19
53	First-principles study of a hybrid carbon material: Imperfect fullerenes covalently bonded to defective single-walled carbon nanotubes. *Physical Review B*, **2008**, 77,	3.3	19
52	Vacancy-assisted diffusion mechanism of group-III elements in ZnO: An ab initio study. *Journal of Applied Physics*, **2009**, 105, 073504	2.5	18
51	Atomistic study of lattice trapping behavior for brittle fracture in bcc-iron. *Computational Materials Science*, **2007**, 40, 376-381	3.2	18
50	Influence of the alloying elements Re, Co and W on the propagation of the Ni/Ni3Al interface crack. *RSC Advances*, **2015**, 5, 52473-52480	3.7	16
49	Transition-metal alloying of γ′-Ni3Al: Effects on the ideal uniaxial compressive strength from first-principles calculations. *Physical Review B*, **2018**, 97,	3.3	15
48	A first-principles survey of the partitioning behaviors of alloying elements on γ/γ′ interface. *Journal of Applied Physics*, **2008**, 104, 013109	2.5	15
47	Mechanical properties and electronic structure of superhard diamondlike BC5: A first-principles study. *Journal of Applied Physics*, **2009**, 106, 043513	2.5	14
46	Atomistic simulation of fracture in Ni3Al. *Journal of Materials Research*, **2008**, 23, 1597-1603	2.5	14
45	Effect of alloying elements on the ideal strength and charge redistribution of γ′-Ni3Al: a first-principles study of tensile deformation. *RSC Advances*, **2016**, 6, 77489-77498	3.7	14
44	Density functional theory study of the thermodynamic and elastic properties of Ni-based superalloys. *Journal of Physics Condensed Matter*, **2015**, 27, 295401	1.8	13
43	Transition-metal-element dependence of ideal shear strength and elastic behaviors of γ′-Ni3Al: ab initio study to guide rational alloy design. *Journal of Alloys and Compounds*, **2019**, 806, 1260-1266	5.7	13

42	Electronic structure analysis of self-consistent embedding theory for quantum/molecular mechanics simulations. *Physical Review B*, **2008**, 78,	3.3	13
41	Effect of alloying element on dislocation cross-slip in γ-Ni3Al: a first-principles study. *Philosophical Magazine*, **2012**, 92, 4028-4039	1.6	12
40	Effect of Re on lattice trapping in γ-Ni3Al cracks by atomistic simulation. *Computational Materials Science*, **2015**, 97, 102-108	3.2	11
39	A ternary NiAlW EAM potential for Ni-based single crystal superalloys. *Physica B: Condensed Matter*, **2015**, 456, 283-292	2.8	11
38	Effect of the alloying element on the temperature-dependent ideal shear strength of γ-Ni3Al. *RSC Advances*, **2016**, 6, 20551-20558	3.7	10
37	Effect of alloying elements on the elastic properties of γ-Ni and γ-Ni3Al from first-principles calculations. *Materials Research Society Symposia Proceedings*, **2009**, 1224, 1		9
36	First-principles investigation of 3d transition elements in L10 TiAl. *Journal of Applied Physics*, **2007**, 101, 083702	2.5	9
35	Atomistic simulation for configuration evolution and energetic calculation of crack in body-centered-cubic iron. *Journal of Materials Research*, **2006**, 21, 2542-2549	2.5	9
34	First-principles study of Ni/Ni3Al interface doped with Re, Ta and W. *Computational Materials Science*, **2020**, 175, 109586	3.2	8
33	Influence of alloying elements upon the theoretical tensile strength of Ni-based model superalloy: γ-Ni/γ′-Ni3Al multilayer. *Computational Materials Science*, **2016**, 119, 120-129	3.2	7
32	The ternary NiAlCo embedded-atom-method potential for γ′ Ni-based single-crystal superalloys: Construction and application. *Chinese Physics B*, **2014**, 23, 033401	1.2	7
31	Adsorption, diffusion, and site exchange for Ge ad-dimers on Sb-covered Si(001) from first-principles total-energy calculations. *Physical Review B*, **2006**, 74,	3.3	7
30	First-principles study on the effect of impurities at the front of cracks in Fe. *Physical Review B*, **2005**, 72,	3.3	7
29	Electronic structure and multi-scale behaviour for the dislocation–doping complex in the gamma phase of nickel-base superalloys. *RSC Advances*, **2017**, 7, 19124-19135	3.7	6
28	Effect of Re and W upon brittle fracture in Ni3Al cracks by atomic simulation. *Computational Materials Science*, **2015**, 110, 261-269	3.2	6
27	Effect of Re on dislocation nucleation from crack tip in Ni by atomistic simulation. *Computational Materials Science*, **2015**, 97, 127-135	3.2	6
26	Alloying-element dependence of structural, elastic and electronic properties of nickel-based superalloys: Influence of γ′ volume fraction. *Journal of Alloys and Compounds*, **2020**, 838, 155141	5.7	6
25	Electronic structure of edge dislocation of core-doped Ti in Fe. *Progress in Natural Science: Materials International*, **2004**, 14, 477-482	3.6	6

24	Diffusion in Ni-Based Single Crystal Superalloys with Density Functional Theory and Kinetic Monte Carlo Method. *Communications in Computational Physics*, **2016**, 20, 603-618	2.4	6
23	Cross-slip process in model Ni(Al) solid solution: An embedded-atom method study. *Computational Materials Science*, **2014**, 91, 192-199	3.2	5
22	First-principles study for transport properties of armchair carbon nanotubes with a double vacancy under strain. *Journal of Applied Physics*, **2008**, 103, 113714	2.5	5
21	Re effects in model Ni-based superalloys investigated with first-principles calculations and atom probe tomography. *Chinese Physics B*, **2020**, 29, 043103	1.2	4
20	Lattice stability and the effect of Co and Re on the ideal strength of Ni: First-principles study of uniaxial tensile deformation. *Chinese Physics B*, **2017**, 26, 093106	1.2	4
19	Multiscale analysis and numerical algorithm for the Schr□inger equations in heterogeneous media. *Applied Mathematics and Computation*, **2010**, 217, 3955-3973	2.7	4
18	Dependence of mechanical properties on the site occupancy of ternary alloying elements in □-Ni3Al: Ab initio description for shear and tensile deformation. *Chinese Physics B*, **2020**, 29, 078103	1.2	4
17	Compressive behavior and elastic properties of Ni-based □ternary model superalloys: First-principles calculations and rule of mixtures predications. *Journal of Alloys and Compounds*, **2020**, 839, 155661	5.7	3
16	The effects of combining alloying elements on the elastic properties of □-Ni in Ni-based superalloy: High-throughput first-principles calculations. *Chinese Physics B*, **2018**, 27, 077104	1.2	3
15	Dimer-breaking-assisted exchange mechanism in surfactant-mediated epitaxial growth of Ge on Si(001): Ab initio total energy calculations. *Physical Review B*, **2007**, 76,	3.3	3
14	First principles study of the diffusional phenomena across the clean and Re-doped □-Ni/ □-Ni 3 Al interface of Ni-based single crystal superalloy. *Chinese Physics B*, **2016**, 25, 067104	1.2	2
13	Anisotropic elastic properties and ideal uniaxial compressive strength of TiB 2 from first principles calculations. *Chinese Physics B*, **2018**, 27, 077103	1.2	2
12	Effects of Re, W and Co on dislocation nucleation at the crack tip in the -phase of Ni-based single-crystal superalloys by atomistic simulation. *Royal Society Open Science*, **2019**, 6, 190441	3.3	2
11	Synergistic strengthening mechanisms of rhenium in nickel-based single crystal superalloys. *Intermetallics*, **2021**, 132, 107133	3.5	2
10	Construction of ternary Ni□Al□Ta potential and its application in the effect of Ta on [1 1 0] edge dislocation slipping in □(Ni3Al). *Computational Materials Science*, **2016**, 118, 288-296	3.2	2
9	Site preferences of alloying transition metal elements in Ni-based superalloy: A first-principles study. *Chinese Physics B*, **2018**, 27, 097102	1.2	2
8	Construction of Ni□Al□Ru EAM potential and application in misfit dislocation system. *Progress in Natural Science: Materials International*, **2020**, 30, 539-544	3.6	1
7	Effect of Re on stacking fault nucleation under shear strain in Ni by atomistic simulation. *Chinese Physics B*, **2014**, 23, 110208	1.2	1

6	First-Principles Study of the Electronic Properties of γ⁄γ′ Interface in Ni Based Superalloys. *Materials Transactions*, **2005**, 46, 1122-1126	1.3	1
5	Doping effects on the stacking fault energies of the phase in Ni-based superalloys. *Chinese Physics B*, **2020**, 29, 026401	1.2	1
4	Novel structures and mechanical properties of Zr2N: Ab initio description under high pressures. *Chinese Physics B*, **2021**, 30, 016403	1.2	1
3	Transition metal solutes in Ni-based ternary model superalloys: Partitioning and effects on elastic properties from first-principles calculations. *Computational Materials Science*, **2021**, 195, 110447	3.2	0
2	CLUSTER-SIMULATED DISLOCATION CORE: MOTION AND TRAP FOR IMPURITY ATOMS. *International Journal of Modern Physics B*, **2005**, 19, 2353-2358	1.1	
1	Multiscale energy density algorithm and application to surface structure of Ni matrix of superalloy. *Chinese Physics B*, **2018**, 27, 097105	1.2	