Chong-Yu Wang

List of Publications by Year
in descending order

80	1,650	304701	330122
papers	citations	22 h-index	37 g-index

81	81	81	1097
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Predicting creep rupture life of Ni-based single crystal superalloys using divide-and-conquer approach based machine learning. Acta Materialia, 2020, 195, 454-467.	7.9	113
2	The effect of alloying elements on the dislocation climbing velocity in Ni: A first-principles study. Acta Materialia, 2009, 57, 5914-5920.	7.9	81
3	Misfit dislocation networks in theÎ³â^•Î³â€²phase interface of a Ni-based single-crystal superalloy: Molecular dynamics simulations. Physical Review B, 2005, 72, .	3.2	72
4	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, .	3.3	72
5	Energetics and local spin magnetic moment of single3,4dimpurities encapsulated in an icosahedralAu12cage. Physical Review B, 2004, 70, .	3.2	69
6	The effects of alloying elements on generalized stacking fault energies, strength and ductility of Î³â€²-Ni3Al. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2012, 539, 38-41.	5.6	61
7	Effect of Re in Î³ phase, Î³â€²Î³â€² phase and Î³/Î³â€²Î³/Î³â€² interface of Ni-based single-crystal superalloys. Acta Materialia, 2010, 58, 2045-2055.	7.9	55
8	Phase Diagram of Ising Nano-Particles with Cubic Structures. Physica Status Solidi (B): Basic Research, 2002, 232, 254-263.	1.5	51
9	Influence of the alloying element Re on the ideal tensile and shear strength of Î³â€²-Ni3Al. Scripta Materialia, 2009, 61, 197-200.	5.2	51
10	Energetics and electronic structure of Re and Ta in theÎ³â€²phase of Ni-based superalloys. Physical Review B, 2001, 65, .	3.2	50
11	Ni/Ni3Al interface: A density functional theory study. Applied Surface Science, 2009, 255, 3669-3675.	6.1	49
12	Partitioning and diffusion of transition metal solutes in ternary model Ni-based single crystal superalloys. Materials and Design, 2017, 130, 157-165.	7.0	46
13	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.	5.6	42
14	First-principles study of the stability of the icosahedralTi13,Ti13â^'1,andTi13+1clusters. Physical Review B, 2002, 65, .	3.2	41
15	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.	2.0	37
16	First-principle investigation of 3d transition metal elements in Î³â€²-Co3(Al,W). Journal of Applied Physics, 2010, 107, .	2.5	35
17	Density functional theory study of Ni/Ni3Al interface alloying with Re and Ru. Surface Science, 2008, 602, 2604-2609.	1.9	31
18	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.	2.0	31

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19	Effect of interactions between elements on the diffusion of solutes in Ni X Y systems and Î³â€²-coarsening in model Ni-based superalloys. Scripta Materialia, 2017, 138, 100-104.	5.2	30
20	First-principles study of point defects in solar cell semiconductor CuI. Physica B: Condensed Matter, 2013, 413, 116-119.	2.7	29
21	Electronic states and doping effect of carbon in the edge-dislocation core of bcc iron. Physical Review B, 2004, 69, .	3.2	24
22	First-principles study of contact between Ti surface and semiconducting carbon nanotube. Journal of Applied Physics, 2007, 102, 013709.	2.5	24
23	Molecular dynamics simulations of influence of Re on lattice trapping and fracture stress of cracks in Ni. Computational Materials Science, 2014, 83, 196-206.	3.0	24
24	First-principles study of a hybrid carbon material: Imperfect fullerenes covalently bonded to defective single-walled carbon nanotubes. Physical Review B, 2008, 77, .	3.2	22
25	Influence of alloying elements on the elastic properties of ternary and quaternary nickel-base superalloys. Philosophical Magazine, 2009, 89, 2935-2947.	1.6	22
26	First-principles study of Ni/Ni3Al interface doped with Re, Ta and W. Computational Materials Science, 2020, 175, 109586.	3.0	22
27	Transition-metal alloying of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msup><mml:mi>Î³</mml:mi><mml:mo>â€²</mml:mo></m : Effects on the ideal uniaxial compressive strength from first-principles calculations. Physical Review B, 2018, 97, .	3.2	21
28	Effect of alloying element on dislocation cross-slip in Î³â€²-Ni₃Al: a first-principles study. Philosophical Magazine, 2012, 92, 4028-4039.	1.6	20
29	Influence of the alloying elements Re, Co and W on the propagation of the Ni/Ni₃Al interface crack. RSC Advances, 2015, 5, 52473-52480.	3.6	20
30	Atomistic study of lattice trapping behavior for brittle fracture in bcc-iron. Computational Materials Science, 2007, 40, 376-381.	3.0	19
31	Vacancy-assisted diffusion mechanism of group-III elements in ZnO: An ab initio study. Journal of Applied Physics, 2009, 105, 073504.	2.5	18
32	A ternary Niâ€“Alâ€“W EAM potential for Ni-based single crystal superalloys. Physica B: Condensed Matter, 2015, 456, 283-292.	2.7	17
33	Effect of alloying elements on the ideal strength and charge redistribution of Î³â€²-Ni₃Al: a first-principles study of tensile deformation. RSC Advances, 2016, 6, 77489-77498.	3.6	17
34	Transition-metal-element dependence of ideal shear strength and elastic behaviors of Î³â€²-Ni3Al: ab initio study to guide rational alloy design. Journal of Alloys and Compounds, 2019, 806, 1260-1266.	5.5	17
35	Density functional theory study of the thermodynamic and elastic properties of Ni-based superalloys. Journal of Physics Condensed Matter, 2015, 27, 295401.	1.8	16
36	A first-principles survey of the partitioning behaviors of alloying elements on Î³/Î³â€² interface. Journal of Applied Physics, 2008, 104, 013109.	2.5	15

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37	Synergistic strengthening mechanisms of rhenium in nickel-based single crystal superalloys. Intermetallics, 2021, 132, 107133.	3.9	15
38	Atomistic simulation of fracture in Ni₃Al. Journal of Materials Research, 2008, 23, 1597-1603.	2.6	14
39	Electronic structure analysis of self-consistent embedding theory for quantum/molecular mechanics simulations. Physical Review B, 2008, 78, .	3.2	14
40	Mechanical properties and electronic structure of superhard diamondlike BC5: A first-principles study. Journal of Applied Physics, 2009, 106, .	2.5	14
41	Alloying-element dependence of structural, elastic and electronic properties of nickel-based superalloys: Influence of Î³â€™ volume fraction. Journal of Alloys and Compounds, 2020, 838, 155141.	5.5	14
42	Effect of Re on lattice trapping in Î³â€²-Ni3Al cracks by atomistic simulation. Computational Materials Science, 2015, 97, 102-108.	3.0	13
43	Effect of the alloying element on the temperature-dependent ideal shear strength of Î³â€²-Ni3Al. RSC Advances, 2016, 6, 20551-20558.	3.6	13
44	Atomistic simulation for configuration evolution and energetic calculation of crack in body-centered-cubic iron. Journal of Materials Research, 2006, 21, 2542-2549.	2.6	11
45	The ternary Niâ€”Alâ€”Co embedded-atom-method potential for Î³/Î³â€² Ni-based single-crystal superalloys: Construction and application. Chinese Physics B, 2014, 23, 033401.	1.4	11
46	Influence of alloying elements upon the theoretical tensile strength of Ni-based model superalloy: Î³-Ni/Î³â€²-Ni3Al multilayer. Computational Materials Science, 2016, 119, 120-129.	3.0	11
47	First-principles investigation of 3d transition elements in L10 TiAl. Journal of Applied Physics, 2007, 101, 083702.	2.5	10
48	Effect of Alloying Elements on the Elastic Properties of Î³-Ni and Î³'-Ni3Al from First-principles Calculations. Materials Research Society Symposia Proceedings, 2009, 1224, 1.	0.1	10
49	Effect of Re on dislocation nucleation from crack tip in Ni by atomistic simulation. Computational Materials Science, 2015, 97, 127-135.	3.0	9
50	Diffusion in Ni-Based Single Crystal Superalloys with Density Functional Theory and Kinetic Monte Carlo Method. Communications in Computational Physics, 2016, 20, 603-618.	1.7	9
51	Electronic structure of edge dislocation of core-doped Ti in Fe*. Progress in Natural Science: Materials International, 2004, 14, 477-482.	4.4	7
52	First-principles study on the effect of impurities at the front of cracks inÎ±â€™Fe. Physical Review B, 2005, 72, .	3.2	7
53	Adsorption, diffusion, and site exchange for Ge ad-dimers on Sb-coveredSi(001)from first-principles total-energy calculations. Physical Review B, 2006, 74, .	3.2	7
54	Cross-slip process in model Ni(Al) solid solution: An embedded-atom method study. Computational Materials Science, 2014, 91, 192-199.	3.0	7

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55	Effect of Re and W upon brittle fracture in Ni3Al cracks by atomic simulation. Computational Materials Science, 2015, 110, 261-269.	3.0	7
56	Electronic structure and multi-scale behaviour for the dislocationâ€“doping complex in the gamma phase of nickel-base superalloys. RSC Advances, 2017, 7, 19124-19135.	3.6	7
57	Compressive behavior and elastic properties of Ni-based Î³/Î³â€™ ternary model superalloys: First-principles calculations and rule of mixtures predications. Journal of Alloys and Compounds, 2020, 839, 155661.	5.5	7
58	First principles study of the diffusional phenomena across the clean and Re-doped Î³ -Ni/ Î³ â€™-Ni ₃ Al interface of Ni-based single crystal superalloy. Chinese Physics B, 2016, 25, 067104.	1.4	6
59	The effects of combining alloying elements on the elastic properties of Î³ -Ni in Ni-based superalloy: High-throughput first-principles calculations. Chinese Physics B, 2018, 27, 077104.	1.4	6
60	Effects of Re, W and Co on dislocation nucleation at the crack tip in the Î³ -phase of Ni-based single-crystal superalloys by atomistic simulation. Royal Society Open Science, 2019, 6, 190441.	2.4	6
61	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
62	Multiscale analysis and numerical algorithm for the SchrÃ¶dinger equations in heterogeneous media. Applied Mathematics and Computation, 2010, 217, 3955-3973.	2.2	4
63	Construction of ternary Niâ€“Alâ€“Ta potential and its application in the effect of Ta on [1 1 0] edge dislocation slipping in Î³â€²(Ni3Al). Computational Materials Science, 2016, 118, 288-296.	3.0	4
64	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.	1.4	4
65	Dependence of mechanical properties on the site occupancy of ternary alloying elements in Î³â€²-Ni3Al: Ab initio description for shear and tensile deformation. Chinese Physics B, 2020, 29, 078103.	1.4	4
66	Construction of Niâ€“Alâ€“Ru EAM potential and application in misfit dislocation system. Progress in Natural Science: Materials International, 2020, 30, 539-544.	4.4	4
67	Re effects in model Ni-based superalloys investigated with first-principles calculations and atom probe tomography*. Chinese Physics B, 2020, 29, 043103.	1.4	4
68	Dimer-breaking-assisted exchange mechanism in surfactant-mediated epitaxial growth of Ge on Si(001):Ab initiototal energy calculations. Physical Review B, 2007, 76, .	3.2	3
69	Site preferences of alloying transition metal elements in Ni-based superalloy: A first-principles study. Chinese Physics B, 2018, 27, 097102.	1.4	3
70	Anisotropic elastic properties and ideal uniaxial compressive strength of TiB 2 from first principles calculations. Chinese Physics B, 2018, 27, 077103.	1.4	3
71	Doping effects on the stacking fault energies of the Î³â€² phase in Ni-based superalloys. Chinese Physics B, 2020, 29, 026401.	1.4	3
72	Novel structures and mechanical properties of Zr₂N: Ab initio description under high pressures*. Chinese Physics B, 2021, 30, 016403.	1.4	3

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73	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.	3.0	3
74	The effect of Ta, W, and Re additions on the tensile-deformation behavior of model Ni-based single-crystal superalloys at intermediate temperature. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2022, 850, 143594.	5.6	2
75	First-Principles Study of the Electronic Properties of γ⁄γ′ Interface in Ni Based Superalloys. Materials Transactions, 2005, 46, 1122-1126.	1.2	1
76	Effect of Re on stacking fault nucleation under shear strain in Ni by atomistic simulation. Chinese Physics B, 2014, 23, 110208.	1.4	1
77	CLUSTER-SIMULATED DISLOCATION CORE: MOTION AND TRAP FOR IMPURITY ATOMS. International Journal of Modern Physics B, 2005, 19, 2353-2358.	2.0	0
78	Multiscale energy density algorithm and application to surface structure of Ni matrix of superalloy. Chinese Physics B, 2018, 27, 097105.	1.4	0
79	Modeling the Parallel Efficiency of Density Functional Theory Based Jobs on Sunway TaihuLight. , 2019, , .		0
80	Inter-Job Scheduling of High-Throughput Material Screening Applications. , 2020, , .		0