Duc Nguyen-Manh

List of Publications by Year
in descending order

66 papers	4,303 citations	159585 30 h-index	118850 62 g-index
66 all docs	66 docs citations	66 times ranked	2996 citing authors

#	Article	IF	Citations
1	In situ neutron diffraction unravels deformation mechanisms of a strong and ductile FeCrNi medium entropy alloy. Journal of Materials Science and Technology, 2022, 116, 103-120.	10.7	16
2	Interaction of transmutation products with precipitates, dislocations and grain boundaries in neutron irradiated W. Materialia, 2022, 22, 101370.	2.7	17
3	Generalized universal equation of states for magnetic materials: A novel formulation for an interatomic potential in Fe. Physical Review Materials, 2022, 6, .	2.4	0
4	Mechanical characterisation of V-4Cr-4Ti alloy: Tensile tests under high energy synchrotron diffraction. Journal of Nuclear Materials, 2022, 569, 153911.	2.7	3
5	Effect of axial molecules and linker length on CO₂ adsorption and selectivity of CAU-8: a combined DFT and GCMC simulation study. RSC Advances, 2021, 11, 12460-12469.	3.6	0
6	Composition Stability and Cr-Rich Phase Formation in W-Cr-Y and W-Cr-Ti Smart Alloys. Metals, 2021, 11, 743.	2.3	4
7	Elastic dipole tensors and relaxation volumes of point defects in concentrated random magnetic Fe-Cr alloys. Computational Materials Science, 2021, 194, 110435.	3.0	24
8	First-principles model for voids decorated by transmutation solutes: Short-range order effects and application to neutron irradiated tungsten. Physical Review Materials, 2021, 5, .	2.4	7
9	Advanced Self-Passivating Alloys for an Application under Extreme Conditions. Metals, 2021, 11, 1255.	2.3	12
10	Development of a solute and defect concentration dependant Ising model for the study of transmutation induced segregation in neutron irradiated Wâ€“(Re, Os) systems. Journal of Physics Condensed Matter, 2021, 33, 475902.	1.8	5
11	High-dose ion irradiation damage in Fe28Ni28Mn26Cr18 characterised by TEM and depth-sensing nanoindentation. Nuclear Materials and Energy, 2021, 28, 101028.	1.3	3
12	Mechano-chemical stability and water effect on gas selectivity in mixed-metal zeolitic imidazolate frameworks: a systematic investigation from van der Waals corrected density functional theory. Physical Chemistry Chemical Physics, 2020, 22, 1598-1610.	2.8	1
13	Chemical short-range order in derivative Crâ€“Taâ€“Tiâ€“Vâ€“W high entropy alloys from the first-principles thermodynamic study. Physical Chemistry Chemical Physics, 2020, 22, 23929-23951.	2.8	45
14	The electronic structures and magnetic properties of mixed-valence Fe-based metalâ€“organic VNU-15 frameworks: a theoretical study from linear response DFT+U calculations. RSC Advances, 2020, 10, 34690-34701.	3.6	1
15	Phase stability and magnetic properties in fcc Fe-Cr-Mn-Ni alloys from first-principles modeling. Physical Review B, 2020, 101, .	3.2	30
16	Smart Tungsten-based Alloys for a First Wall of DEMO. Fusion Engineering and Design, 2020, 159, 111742.	1.9	13
17	Quantum de-trapping and transport of heavy defects in tungsten. Nature Materials, 2020, 19, 508-511.	27.5	20
18	Hydrogen adsorption mechanism of MOF-74 metalâ€“organic frameworks: an insight from first principles calculations. RSC Advances, 2020, 10, 43940-43949.	3.6	13

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19	Radiation-induced segregation in W-Re: from kinetic Monte Carlo simulations to atom probe tomography experiments. European Physical Journal B, 2019, 92, 1.	1.5	15
20	Relaxation volumes of microscopic and mesoscopic irradiation-induced defects in tungsten. Journal of Applied Physics, 2019, 126, .	2.5	35
21	Decoration of voids with rhenium and osmium transmutation products in neutron irradiated single crystal tungsten. Scripta Materialia, 2019, 173, 96-100.	5.2	41
22	Outstanding radiation resistance of tungsten-based high-entropy alloys. Science Advances, 2019, 5, eaav2002.	10.3	360
23	Configurational Entropy in Multicomponent Alloys: Matrix Formulation from Ab Initio Based Hamiltonian and Application to the FCC Cr-Fe-Mn-Ni System. Entropy, 2019, 21, 68.	2.2	24
24	Electron delocalization in single-layer phthalocyanine-based covalent organic frameworks: a first principle study. RSC Advances, 2019, 9, 29440-29447.	3.6	11
25	Monitoring Mechanical, Electronic, and Catalytic Trends in a Titanium Metal Organic Framework Under the Influence of Guest-Molecule Encapsulation Using Density Functional Theory. Scientific Reports, 2018, 8, 16651.	3.3	12
26	From Reticular Chemistry Design to Density Functional Theory Modeling for New Zeolitic Imidazolate Framework Topologies: Mechanical Stability, Electronic Structure, and CO₂ Selectivity. Journal of Physical Chemistry C, 2018, 122, 23543-23553.	3.1	4
27	Nano-sized prismatic vacancy dislocation loops and vacancy clusters in tungsten. Nuclear Materials and Energy, 2018, 16, 60-65.	1.3	20
28	The Effect of Electronic Structure on the Phases Present in High Entropy Alloys. Scientific Reports, 2017, 7, 39803.	3.3	54
29	A first-principles model for anomalous segregation in dilute ternary tungsten-rhenium-vacancy alloys. Journal of Physics Condensed Matter, 2017, 29, 145403.	1.8	49
30	Interplay of electronic, structural and magnetic properties as the driving feature of high-entropy CoCrFeNiPd alloys. Journal Physics D: Applied Physics, 2017, 50, 185002.	2.8	16
31	Simulation and Modeling in High Entropy Alloys. Jom, 2017, 69, 2137-2149.	1.9	28
32	Short-Range Order in High Entropy Alloys: Theoretical Formulation and Application to Mo-Nb-Ta-V-W System. Journal of Phase Equilibria and Diffusion, 2017, 38, 391-403.	1.4	102
33	An empirical potential for simulating vacancy clusters in tungsten. Journal of Physics Condensed Matter, 2017, 29, 505501.	1.8	45
34	Magnetic cluster expansion model for random and ordered magnetic face-centered cubic Fe-Ni-Cr alloys. Journal of Applied Physics, 2016, 120, 043902.	2.5	19
35	First-principles modeling of 3d-transition-metal-atom adsorption on silicene: a linear-response DFTâ€‰â€‰+â€‰â€‰Uapproach. Journal of Physics Condensed Matter, 2016, 28, 135301.	1.8	13
36	Phase stability of ternary fcc and bcc Fe-Cr-Ni alloys. Physical Review B, 2015, 91, .	3.2	114

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37	Lattice swelling and modulus change in a helium-implanted tungsten alloy: X-ray micro-diffraction, surface acoustic wave measurements, and multiscale modelling. Acta Materialia, 2015, 89, 352-363.	7.9	123
38	Trapping of He clusters by inert-gas impurities in tungsten: First-principles predictions and experimental validation. Nuclear Instruments & Methods in Physics Research B, 2015, 352, 86-91.	1.4	45
39	Interatomic spacing distribution in multicomponent alloys. Acta Materialia, 2015, 97, 156-169.	7.9	92
40	Constrained non-collinear magnetism in disordered Fe and Feâ€“Cr alloys. Annals of Nuclear Energy, 2015, 77, 246-251.	1.8	8
41	Magnetic and thermodynamic properties of face-centered cubic Feâ€“Ni alloys. Physical Chemistry Chemical Physics, 2014, 16, 16049.	2.8	54
42	Engineering of Band Gap in Metalâ€“Organic Frameworks by Functionalizing Organic Linker: A Systematic Density Functional Theory Investigation. Journal of Physical Chemistry C, 2014, 118, 4567-4577.	3.1	97
43	Neutron-induced dpa, transmutations, gas production, and helium embrittlement of fusion materials. Journal of Nuclear Materials, 2013, 442, S755-S760.	2.7	122
44	First-principles model for phase stability, radiation defects and elastic properties Of Wâ€“Ta and Wâ€“V alloys. Journal of Nuclear Materials, 2013, 442, S680-S683.	2.7	28
45	Recent progress in research on tungsten materials for nuclear fusion applications in Europe. Journal of Nuclear Materials, 2013, 432, 482-500.	2.7	610
46	First-principles models for phase stability and radiation defects in structural materials for future fusion power-plant applications. Journal of Materials Science, 2012, 47, 7385-7398.	3.7	26
47	Phase stability, point defects, and elastic properties of W-V and W-Ta alloys. Physical Review B, 2011, 84, .	3.2	139
48	Review on the EFDA programme on tungsten materials technology and science. Journal of Nuclear Materials, 2011, 417, 463-467.	2.7	157
49	Efficient self-consistency for magnetic tight binding. Computer Physics Communications, 2011, 182, 1350-1360.	7.5	14
50	Magnetic Bond-Order Potential for Iron. Physical Review Letters, 2011, 106, 246402.	7.8	88
51	Magnetic cluster expansion model for bcc-fcc transitions in Fe and Fe-Cr alloys. Physical Review B, 2010, 81, .	3.2	111
52	Magnetic cluster expansion simulations of FeCr alloys. Journal of Nuclear Materials, 2009, 386-388, 22-25.	2.7	43
53	Model many-body Stoner Hamiltonian for binary FeCr alloys. Physical Review B, 2009, 80, .	3.2	29
54	The Feâ€“Cr system: atomistic modelling of thermodynamics and kinetics of phase transformations. Comptes Rendus Physique, 2008, 9, 379-388.	0.9	60

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55	Peierls Potential for Crowdions in the bcc Transition Metals. Physical Review Letters, 2008, 101, 115504.	7.8	48
56	Monte Carlo study of thermodynamic properties and clustering in the bcc Fe-Cr system. Physical Review B, 2007, 75, .	3.2	121
57	Bond-order potential for simulations of extended defects in tungsten. Physical Review B, 2007, 75, .	3.2	110
58	Environmental dependence of bonding: A challenge for modelling of intermetallics and fusion materials. Progress in Materials Science, 2007, 52, 255-298.	32.8	64
59	Systematic group-specific trends for point defects in bcc transition metals: An ab initio study. Journal of Nuclear Materials, 2007, 367-370, 257-262.	2.7	35
60	Multiscale modeling of crowdion and vacancy defects in body-centered-cubic transition metals. Physical Review B, 2007, 76, .	3.2	396
61	Magnetic origin of nano-clustering and point defect interaction in Feâ€“Cr alloys: an ab-initio study. Journal of Computer-Aided Materials Design, 2007, 14, 159-169.	0.7	39
62	Self-interstitial atom defects in bcc transition metals: Group-specific trends. Physical Review B, 2006, 73, .	3.2	360
63	Magnetic properties of point defects in iron within the tight-binding-bond Stoner model. Physical Review B, 2005, 71, .	3.2	50
64	Electronic origin of structural trends across early transition-metal disilicides: Anomalous behavior ofCrSi2. Physical Review B, 2004, 69, .	3.2	31
65	Ab-Initio Modelling of Point Defect-Impurity Interaction in Tungsten and other BCC Transition Metals. Advanced Materials Research, 0, 59, 253-256.	0.3	26
66	<i>Ab Initio</i> Based Modelling of Diffusion and Phase Stability of Alloys. , 0, 12, 1-22.		1