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	Recent progress in research on tungsten materials for nuclear fusion applications in Europe. Journal of Nuclear Materials, 2013, 432, 482-500.	2.7	610
2	Multiscale modeling of crowdion and vacancy defects in body-centered-cubic transition metals. Physical Review B, 2007, 76, .	3.2	396
3	Self-interstitial atom defects in bcc transition metals: Group-specific trends. Physical Review B, 2006, 73, .	3.2	360
4	Outstanding radiation resistance of tungsten-based high-entropy alloys. Science Advances, 2019, 5, eaav2002.	10.3	360
5	Review on the EFDA programme on tungsten materials technology and science. Journal of Nuclear Materials, 2011, 417, 463-467.	2.7	157
6	Phase stability, point defects, and elastic properties of W-V and W-Ta alloys. Physical Review B, 2011, 84, .	3.2	139
7	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
8	Neutron-induced dpa, transmutations, gas production, and helium embrittlement of fusion materials. Journal of Nuclear Materials, 2013, 442, S755-S760.	2.7	122
9	Monte Carlo study of thermodynamic properties and clustering in the bcc Fe-Cr system. Physical Review B, 2007, 75, .	3.2	121
10	Phase stability of ternary fcc and bcc Fe-Cr-Ni alloys. Physical Review B, 2015, 91, .	3.2	114
11	Magnetic cluster expansion model for bcc-fcc transitions in Fe and Fe-Cr alloys. Physical Review B, 2010, 81, .	3.2	111
12	Bond-order potential for simulations of extended defects in tungsten. Physical Review B, 2007, 75, .	3.2	110
13	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
14	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
15	Interatomic spacing distribution in multicomponent alloys. Acta Materialia, 2015, 97, 156-169.	7.9	92
16	Magnetic Bond-Order Potential for Iron. Physical Review Letters, 2011, 106, 246402.	7.8	88
17	Environmental dependence of bonding: A challenge for modelling of intermetallics and fusion materials. Progress in Materials Science, 2007, 52, 255-298.	32.8	64
18	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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19	Magnetic and thermodynamic properties of face-centered cubic Feâ€“Ni alloys. Physical Chemistry Chemical Physics, 2014, 16, 16049.	2.8	54
20	The Effect of Electronic Structure on the Phases Present in High Entropy Alloys. Scientific Reports, 2017, 7, 39803.	3.3	54
21	Magnetic properties of point defects in iron within the tight-binding-bond Stoner model. Physical Review B, 2005, 71, .	3.2	50
22	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
23	Peierls Potential for Crowdions in the bcc Transition Metals. Physical Review Letters, 2008, 101, 115504.	7.8	48
24	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
25	An empirical potential for simulating vacancy clusters in tungsten. Journal of Physics Condensed Matter, 2017, 29, 505501.	1.8	45
26	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
27	Magnetic cluster expansion simulations of FeCr alloys. Journal of Nuclear Materials, 2009, 386-388, 22-25.	2.7	43
28	Decoration of voids with rhenium and osmium transmutation products in neutron irradiated single crystal tungsten. Scripta Materialia, 2019, 173, 96-100.	5.2	41
29	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
30	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
31	Relaxation volumes of microscopic and mesoscopic irradiation-induced defects in tungsten. Journal of Applied Physics, 2019, 126, .	2.5	35
32	Electronic origin of structural trends across early transition-metal disilicides: Anomalous behavior ofCrSi2. Physical Review B, 2004, 69, .	3.2	31
33	Phase stability and magnetic properties in fcc Fe-Cr-Mn-Ni alloys from first-principles modeling. Physical Review B, 2020, 101, .	3.2	30
34	Model many-body Stoner Hamiltonian for binary FeCr alloys. Physical Review B, 2009, 80, .	3.2	29
35	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
36	Simulation and Modeling in High Entropy Alloys. Jom, 2017, 69, 2137-2149.	1.9	28

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37	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
38	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
39	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
40	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
41	Nano-sized prismatic vacancy dislocation loops and vacancy clusters in tungsten. Nuclear Materials and Energy, 2018, 16, 60-65.	1.3	20
42	Quantum de-trapping and transport of heavy defects in tungsten. Nature Materials, 2020, 19, 508-511.	27.5	20
43	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
44	Interaction of transmutation products with precipitates, dislocations and grain boundaries in neutron irradiated W. Materialia, 2022, 22, 101370.	2.7	17
45	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
46	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
47	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
48	Efficient self-consistency for magnetic tight binding. Computer Physics Communications, 2011, 182, 1350-1360.	7.5	14
49	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
50	Smart Tungsten-based Alloys for a First Wall of DEMO. Fusion Engineering and Design, 2020, 159, 111742.	1.9	13
51	Hydrogen adsorption mechanism of MOF-74 metalâ€“organic frameworks: an insight from first principles calculations. RSC Advances, 2020, 10, 43940-43949.	3.6	13
52	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
53	Advanced Self-Passivating Alloys for an Application under Extreme Conditions. Metals, 2021, 11, 1255.	2.3	12
54	Electron delocalization in single-layer phthalocyanine-based covalent organic frameworks: a first principle study. RSC Advances, 2019, 9, 29440-29447.	3.6	11

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55	Constrained non-collinear magnetism in disordered Fe and Feâ€“Cr alloys. Annals of Nuclear Energy, 2015, 77, 246-251.	1.8	8
56	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
57	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
58	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
59	Composition Stability and Cr-Rich Phase Formation in W-Cr-Y and W-Cr-Ti Smart Alloys. Metals, 2021, 11, 743.	2.3	4
60	High-dose ion irradiation damage in Fe28Ni28Mn26Cr18 characterised by TEM and depth-sensing nanoindentation. Nuclear Materials and Energy, 2021, 28, 101028.	1.3	3
61	Mechanical characterisation of V-4Cr-4Ti alloy: Tensile tests under high energy synchrotron diffraction. Journal of Nuclear Materials, 2022, 569, 153911.	2.7	3
62	<i>Ab Initio</i> Based Modelling of Diffusion and Phase Stability of Alloys. , 0, 12, 1-22.		1
63	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
64	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
65	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
66	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