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List of Publications by Year
in descending order

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57 papers	1,937 citations	257357 24 h-index	254106 43 g-index
58 all docs	58 docs citations	58 times ranked	1845 citing authors

#	Article	IF	Citations
1	First-principles study of the structural, electronic, vibrational, and elastic properties of orthorhombic NiSi. Physical Review B, 2009, 79, .	1.1	202
2	Role of the Dopant in the Superconductivity of Diamond. Physical Review Letters, 2004, 93, 237004.	2.9	164
3	Room Temperature Peierls Distortion in Small Diameter Nanotubes. Physical Review Letters, 2005, 94, 015503.	2.9	140
4	Superconductivity in Dopedsp3Semiconductors: The Case of the Clathrates. Physical Review Letters, 2003, 91, 247001.	2.9	136
5	First principle calculations of the Î¹-Fe3AlC perovskite and ironâ€“aluminium intermetallics. Intermetallics, 2008, 16, 345-352.	1.8	72
6	Stability of vacancy-hydrogen clusters in nickel from first-principles calculations. Acta Materialia, 2014, 78, 135-143.	3.8	70
7	Pressure stability and low compressibility of intercalated cagelike materials: The case of silicon clathrates. Physical Review B, 2002, 65, .	1.1	66
8	Tailoring Band Gap and Hardness by Intercalation: Anab initioStudy ofI8@Siâ˜†46and Related Doped Clathrates. Physical Review Letters, 2001, 87, 206405.	2.9	64
9	Effect of trapping and temperature on the hydrogen embrittlement susceptibility of alloy 718. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2014, 611, 370-382.	2.6	63
10	A Calphad assessment of Alâ€“Câ€“Fe system with the carbide modelled as an ordered form of the fcc phase. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2008, 32, 361-370.	0.7	60
11	First-principles study of nickel-silicides ordered phases. Journal of Alloys and Compounds, 2011, 509, 2639-2644.	2.8	52
12	First-principles study of diffusion and interactions of vacancies and hydrogen in hcp-titanium. Journal of Physics Condensed Matter, 2011, 23, 405401.	0.7	51
13	Segregation of hydrogen to defects in nickel using first-principles calculations: The case of self-interstitials and cavities. Journal of Alloys and Compounds, 2014, 614, 211-220.	2.8	46
14	First principle energies of binary and ternary phases of the Feâ€“Nbâ€“Niâ€“Cr system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2011, 35, 588-593.	0.7	41
15	First-principles nickel database: Energetics of impurities and defects. Computational Materials Science, 2015, 101, 77-87.	1.4	40
16	Calphad-type assessment of the Feâ€“Nbâ€“Ni ternary system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2009, 33, 136-161.	0.7	39
17	Influence of trap connectivity on H diffusion: Vacancy trapping. Acta Materialia, 2016, 103, 334-340.	3.8	38
18	Guest displacement in silicon clathrates. Physical Review B, 2004, 69, .	1.1	36

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19	Structural and electronic properties ofp-doped silicon clathrates. Physical Review B, 2007, 75, .	1.1	34
20	First-principles calculations of carbon clathrates: Comparison to silicon and germanium clathrates. Physical Review B, 2010, 82, .	1.1	34
21	Elastic properties of the Î±' martensitic phase in the Ti-6Al-4V alloy obtained by additive manufacturing. Scripta Materialia, 2019, 167, 115-119.	2.6	32
22	First-principles study of transition metal carbides. Materials Research Express, 2016, 3, 126502.	0.8	30
23	Atomistic modelling of hydrogen segregation to the Î£9{2 2 1}[1 1 0] symmetric tilt grain boundary in Al. Philosophical Magazine, 2014, 94, 2247-2261.	0.7	29
24	Dislocation/hydrogen interaction mechanisms in hydrided nanocrystalline palladium films. Acta Materialia, 2016, 111, 253-261.	3.8	28
25	Carbon cage-like materials as potential low work function metallic compounds: Case of clathrates. Applied Physics Letters, 2002, 80, 1385-1387.	1.5	25
26	Stress-controlled carbon diffusion channeling in bct-iron: A mean-field theory. Journal of Alloys and Compounds, 2018, 769, 1121-1131.	2.8	23
27	Electronic and superconducting properties of silicon and carbon clathrates. Applied Surface Science, 2004, 226, 289-297.	3.1	20
28	Study of multivacancies in alpha Fe. Journal of Nuclear Materials, 2013, 441, 168-177.	1.3	20
29	First-principles study of sulfur multi-absorption in nickel and its segregation to the Ni(100) and Ni(111) surfaces. Surface Science, 2013, 617, 15-21.	0.8	19
30	Hydrogen influence on diffusion in nickel from first-principles calculations. Physical Review B, 2015, 91, .	1.1	19
31	Effect of stress on vacancy formation and diffusion in fcc systems: Comparison between DFT calculations and elasticity theory. Acta Materialia, 2020, 200, 869-882.	3.8	18
32	DFT study of the solubility of hydrogen and carbon in <mml:math altimg="si28.gif" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd" xmlns:ce="h. Journal of Alloys and Co.	2.8	16
33	Diffusion and segregation of niobium in fcc-nickel. Journal of Physics Condensed Matter, 2012, 24, 095010.	0.7	15
34	Effects of impurities on graphite shape during solidification of spheroidal graphite cast ions. Materialia, 2019, 8, 100471.	1.3	15
35	Theoretical study on hydrogen solubility and diffusivity in the Î³-TiAl L10 structure. International Journal of Hydrogen Energy, 2019, 44, 12215-12227.	3.8	15
36	Diffusion of interstitial species (H and O atoms) in fcc systems (Al, Cu, Co, Ni and Pd): Contribution of first and second order transition states. Journal of Alloys and Compounds, 2019, 772, 280-287.	2.8	15

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37	Nickel isotope fractionation during metal-silicate differentiation of planetesimals: Experimental petrology and ab initio calculations. Geochimica Et Cosmochimica Acta, 2020, 269, 238-256.	1.6	15
38	Diffusion of interstitials in metallic systems, illustration of a complex study case: aluminum. Journal of Physics Condensed Matter, 2017, 29, 455703.	0.7	14
39	First-principles study of the insertion and diffusion of interstitial atoms (H, C, N and O) in nickel. Journal of Alloys and Compounds, 2020, 822, 153555.	2.8	14
40	Impact of the clusterization on the solubility of oxygen and vacancy concentration in nickel: A multi-scale approach. Journal of Alloys and Compounds, 2017, 708, 1063-1072.	2.8	12
41	Atomic-scale study of low-temperature equilibria in iron-rich Al-C-Fe. Physical Review B, 2008, 78, .	1.1	11
42	Study of vacancy-(H,B,C,N,O) clusters in Al using DFT and statistical approaches: Consequences on solubility of solutes. Journal of Alloys and Compounds, 2018, 748, 12-25.	2.8	11
43	Theoretical study of the insertion and diffusivity of hydrogen in the Ti3Al-D019 system: Comparison with Ti-hcp and TiAl-L10 systems. International Journal of Hydrogen Energy, 2019, 44, 32307-32322.	3.8	11
44	Stability of Zener order in martensite: an atomistic evidence. Scripta Materialia, 2021, 194, 113632.	2.6	9
45	Theoretical study of oxygen insertion and diffusivity in theg-TiAlL1₀system. Journal of Physics Condensed Matter, 2020, 32, 175702.	0.7	8
46	A New Class of Low Compressibility Materials: Clathrates of Silicon and Related Materials. High Pressure Research, 2002, 22, 539-544.	0.4	7
47	Effect of pentagons in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mi mathvariant="italic">sp</mml:mi><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msup></mml:mrow></mml:math>system on electronic, elastic, and vibrational properties: Case of chiral structures. Physical Review B, 2011, 83, .	1.1	6
48	Segregation of hydrogen and vacancies at the Î£5(210)[001] symmetric tilt grain boundary in Ni and influence on cohesion. Modelling and Simulation in Materials Science and Engineering, 2021, 29, 055004.	0.8	5
49	Hydrogen diffusivity and solubility in stressed fcc crystals. Journal of Alloys and Compounds, 2021, 879, 160425.	2.8	5
50	Lattice instabilities in hexagonal NiSi: A NiAs prototype structure. Physical Review B, 2010, 81, .	1.1	4
51	Site stability and pipe diffusion of hydrogen under localised shear in aluminium. Philosophical Magazine, 2019, 99, 1184-1205.	0.7	4
52	Insertion and diffusion of N and C in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e1022" altimg="si61.svg"><mml:mi>Î³</mml:mi></mml:math>â€“TiAl: Theoretical study and comparison with O. Physica B: Condensed Matter, 2022, 624, 413370.	1.3	4
53	Comparative study of metallic silicideâ€“germanide orthorhombic MnP systems. Journal of Physics Condensed Matter, 2013, 25, 355403.	0.7	3
54	Interactions of oxygen with intrinsic defects in L1<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e1983" altimg="si96.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>0</mml:mn></mml:mrow></mml:msub></mml:math> <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e1991" altimg="si48.svg"><mml:mi>Î³</mml:mi></mml:math>-TiAl in presence of substitutional solutes: Influenc	1.4	3

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55	Investigation of the mechanical properties of MnSi via EBSD-nanoindentation coupling and ab-initio calculation. Journal of Alloys and Compounds, 2022, 900, 163458.	2.8	3
56	Effect of sub-surface hydrogen on intrinsic crack tip plasticity in aluminium. Philosophical Magazine, 2019, 99, 2355-2375.	0.7	1
57	Optimisation of the parameters of an extended defect model applied to non-amorphizing implants. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2005, 124-125, 397-400.	1.7	0