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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	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	1.3	4
2	Interactions of oxygen with intrinsic defects in L<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
3	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
4	Stability of Zener order in martensite: an atomistic evidence. Scripta Materialia, 2021, 194, 113632.	2.6	9
5	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
6	Hydrogen diffusivity and solubility in stressed fcc crystals. Journal of Alloys and Compounds, 2021, 879, 160425.	2.8	5
7	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
8	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
9	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
10	Theoretical study of oxygen insertion and diffusivity in theg-TiAlL1₀system. Journal of Physics Condensed Matter, 2020, 32, 175702.	0.7	8
11	Effects of impurities on graphite shape during solidification of spheroidal graphite cast ions. Materialia, 2019, 8, 100471.	1.3	15
12	Effect of sub-surface hydrogen on intrinsic crack tip plasticity in aluminium. Philosophical Magazine, 2019, 99, 2355-2375.	0.7	1
13	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
14	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
15	Site stability and pipe diffusion of hydrogen under localised shear in aluminium. Philosophical Magazine, 2019, 99, 1184-1205.	0.7	4
16	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
17	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
18	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

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19	Stress-controlled carbon diffusion channeling in bct-iron: A mean-field theory. Journal of Alloys and Compounds, 2018, 769, 1121-1131.	2.8	23
20	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
21	Diffusion of interstitials in metallic systems, illustration of a complex study case: aluminum. Journal of Physics Condensed Matter, 2017, 29, 455703.	0.7	14
22	First-principles study of transition metal carbides. Materials Research Express, 2016, 3, 126502.	0.8	30
23	Dislocation/hydrogen interaction mechanisms in hydrided nanocrystalline palladium films. Acta Materialia, 2016, 111, 253-261.	3.8	28
24	Influence of trap connectivity on H diffusion: Vacancy trapping. Acta Materialia, 2016, 103, 334-340.	3.8	38
25	Hydrogen influence on diffusion in nickel from first-principles calculations. Physical Review B, 2015, 91, .	1.1	19
26	First-principles nickel database: Energetics of impurities and defects. Computational Materials Science, 2015, 101, 77-87.	1.4	40
27	Stability of vacancy-hydrogen clusters in nickel from first-principles calculations. Acta Materialia, 2014, 78, 135-143.	3.8	70
28	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	2.8	16
29	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
30	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
31	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
32	Study of multivacancies in alpha Fe. Journal of Nuclear Materials, 2013, 441, 168-177.	1.3	20
33	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
34	Comparative study of metallic silicideâ€“germanide orthorhombic MnP systems. Journal of Physics Condensed Matter, 2013, 25, 355403.	0.7	3
35	Diffusion and segregation of niobium in fcc-nickel. Journal of Physics Condensed Matter, 2012, 24, 095010.	0.7	15
36	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

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37	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
38	First-principles study of nickel-silicides ordered phases. Journal of Alloys and Compounds, 2011, 509, 2639-2644.	2.8	52
39	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>systems on electronic, elastic, and vibrational properties: Case of chiral structures. Physical Review B, 2011, 83, .	1.1	15
40	Lattice instabilities in hexagonal NiSi: A NiAs prototype structure. Physical Review B, 2010, 81, .	1.1	4
41	First-principles calculations of carbon clathrates: Comparison to silicon and germanium clathrates. Physical Review B, 2010, 82, .	1.1	34
42	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
43	First-principles study of the structural, electronic, vibrational, and elastic properties of orthorhombic NiSi. Physical Review B, 2009, 79, .	1.1	202
44	First principle calculations of the Î¹-Fe3AlC perovskite and ironâ€“aluminium intermetallics. Intermetallics, 2008, 16, 345-352.	1.8	72
45	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
46	Atomic-scale study of low-temperature equilibria in iron-rich Al-C-Fe. Physical Review B, 2008, 78, .	1.1	11
47	Structural and electronic properties ofp-doped silicon clathrates. Physical Review B, 2007, 75, .	1.1	34
48	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
49	Room Temperature Peierls Distortion in Small Diameter Nanotubes. Physical Review Letters, 2005, 94, 015503.	2.9	140
50	Guest displacement in silicon clathrates. Physical Review B, 2004, 69, .	1.1	36
51	Electronic and superconducting properties of silicon and carbon clathrates. Applied Surface Science, 2004, 226, 289-297.	3.1	20
52	Role of the Dopant in the Superconductivity of Diamond. Physical Review Letters, 2004, 93, 237004.	2.9	164
53	Superconductivity in Dopedsp3Semiconductors: The Case of the Clathrates. Physical Review Letters, 2003, 91, 247001.	2.9	136
54	Pressure stability and low compressibility of intercalated cagelike materials: The case of silicon clathrates. Physical Review B, 2002, 65, .	1.1	66

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55	A New Class of Low Compressibility Materials: Clathrates of Silicon and Related Materials. High Pressure Research, 2002, 22, 539-544.	0.4	7
56	Carbon cage-like materials as potential low work function metallic compounds: Case of clathrates. Applied Physics Letters, 2002, 80, 1385-1387.	1.5	25
57	Tailoring Band Gap and Hardness by Intercalation: Anab initioStudy ofI8@Siâˆ'46and Related Doped Clathrates. Physical Review Letters, 2001, 87, 206405.	2.9	64