Andrei V Ruban

List of Publications by Year
in descending order

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102 papers	10,717 citations	61984 43 h-index	43889 91 g-index
102 all docs	102 docs citations	102 times ranked	10404 citing authors

#	Article	IF	Citations
1	Towards predictive simulations of spinodal decomposition in Fe-Cr alloys. Computational Materials Science, 2022, 202, 110955.	3.0	4
2	Ab initio surface free energies of tungsten with full account of thermal excitations. Physical Review B, 2022, 105, .	3.2	10
3	Structural vacancies in (Ti,Al)N: An ab initio study. Physical Review Materials, 2022, 6, .	2.4	1
4	Stability and ordering of bcc and hcp TiAl+Mo phases: An ab initio study. Computational Materials Science, 2022, 205, 111163.	3.0	5
5	Solubility and segregation of B in paramagnetic fcc Fe. Physical Review Materials, 2022, 6, .	2.4	4
6	Ab initio simulations of the surface free energy of TiN(001). Physical Review B, 2021, 103, .	3.2	9
7	Surface energetics of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si35.svg"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="normal">Al</mml:mi></mml:mrow><mml:mrow><mml:mi>x</mml:mi></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">Ti</mml:mi></mml:mrow><mml:mrow><mml:mn>1</mml:mn><mml:mo>-</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math> alloys. Computational Materials Science, 2020, 183, 109813.	3.0	11
8	Performance of the standard exchange-correlation functionals in predicting melting properties fully from first principles: Application to Al and magnetic Ni. Physical Review B, 2020, 101, .	3.2	15
9	Short-range order in face-centered cubic VCoNi alloys. Physical Review Materials, 2020, 4, .	2.4	24
10	Influence of composition and oxygen-vacancy ordering on lattice parameter and elastic moduli of Ce1-Gd O2-/2: A theoretical study. Scripta Materialia, 2019, 158, 126-130.	5.2	7
11	Phase diagram and oxygenâ€“vacancy ordering in the CeO₂â€“Gd₂O₃ system: a theoretical study. Physical Chemistry Chemical Physics, 2018, 20, 11805-11818.	2.8	26
12	Temperature dependence of the stacking-fault Gibbs energy for Al, Cu, and Ni. Physical Review B, 2018, 98, .	3.2	61
13	High-temperature thermophysical properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î³</mml:mi></mml:math> - and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î´</mml:mi></mml:math> -Mn from first principles. Physical Review Materials, 2018, 2, .	2.4	2
14	Evidence for the antiferromagnetic ground state of Zr2TiAl: a first-principles study. Journal of Physics Condensed Matter, 2017, 29, 265801.	1.8	5
15	Deformation Microstructure and Deformation-Induced Martensite in Austenitic Fe-Cr-Ni Alloys Depending on Stacking Fault Energy. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2017, 48, 1-7.	2.2	150
16	Ordering and phase separation in Gd-doped ceria: a combined DFT, cluster expansion and Monte Carlo study. Physical Chemistry Chemical Physics, 2017, 19, 26606-26620.	2.8	23
17	Effect of solution treatment on spinodal decomposition during aging of an Fe-46.5 at.% Cr alloy. Journal of Materials Science, 2017, 52, 326-335.	3.7	17
18	Long-ranged interactions in bcc NbMoTaW high-entropy alloys. Materials Research Letters, 2017, 5, 35-40.	8.7	86

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19	Ab-initio search for cohesion-enhancing solute elements at grain boundaries in molybdenum and tungsten. International Journal of Refractory Metals and Hard Materials, 2016, 60, 75-81.	3.8	82
20	First-principles study of interactions between substitutional solutes in bcc iron. Journal of Nuclear Materials, 2016, 475, 140-148.	2.7	37
21	Revisiting thermodynamics and kinetic diffusivities of uraniumâ€“niobium with Bayesian uncertainty analysis. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2016, 55, 219-230.	1.6	46
22	Effective interactions and atomic ordering in Ni-rich Ni-Re alloys. Physical Review B, 2016, 94, .	3.2	19
23	Magnetic ordering and exchange interactions in structural modifications of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">M</mml:mi><mml:msub><mml:mi mathvariant="normal">n</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mi>Ga</mml:mi></mml:mrow></mml:math>alloys: Interplay of frustration, atomic order, and off-stoichiometry. Physical Review B, 2016, 93, .	3.2	35
24	Direct atom probe tomography observations of concentration fluctuations in Feâ€“Cr solid solution. Scripta Materialia, 2015, 98, 13-15.	5.2	17
25	First-principles study of point defects in Ni₃Al. Philosophical Magazine, 2014, 94, 20-34.	1.6	28
26	Single-site mean-field approach to thermal defects in binary ordered alloys. Philosophical Magazine, 2014, 94, 1192-1201.	1.6	4
27	Vacancy-cluster mechanism of metal-atom diffusion in substoichiometric carbides. Physical Review B, 2013, 87, .	3.2	31
28	Multiscale Approach to Theoretical Simulations of Materials for Nuclear Energy Applications: Fe-Cr and Zr-based Alloys. Materials Research Society Symposia Proceedings, 2013, 1514, 3-14.	0.1	0
29	Importance of Correlation Effects in hcp Iron Revealed by a Pressure-Induced Electronic Topological Transition. Physical Review Letters, 2013, 110, 117206.	7.8	58
30	Stacking-fault energy and anti-Invar effect in Fe-Mn alloy from first principles. Physical Review B, 2012, 86, .	3.2	33
31	Multi-length scale modeling of martensitic transformations in stainless steels. Acta Materialia, 2012, 60, 6508-6517.	7.9	31
32	Ab Initio Study of Advanced Metallic Nuclear Fuels for Fast Breeder Reactors. Materials Research Society Symposia Proceedings, 2012, 1444, 67.	0.1	3
33	Ab Initio Study of Lattice Site Occupancies in Binary Sigma Phases Using a Single-Site Mean Field Model. Applied Sciences (Switzerland), 2012, 2, 654-668.	2.5	11
34	Configurational thermodynamics of the Fe-CrÏƒ phase. Physical Review B, 2011, 84, .	3.2	16
35	Ab initio-based mean-field theory of the site occupation in the Fe-Cr<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Ïƒ</mml:mi></mml:mrow></mml:math>-phase. Physical Review B, 2011, 83, .	3.2	16
36	Effect of Temperature on the Elastic Anisotropy of Pure Fe and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Fe</mml:mi><mml:mn>0.9</mml:mn></mml:msub><mml:msub><mml:mi>Cr</mml:mi><mml:mn> Alloy. Physical Review Letters, 2011, 107, 205504.	7.8	60

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37	Vacancyâ€“solute interactions in ferromagnetic and paramagnetic bcc iron: Ab initio calculations. Journal of Nuclear Materials, 2011, 419, 248-255.	2.7	63
38	First-principles study of elastic properties of Cr- and Fe-rich Fe-Cr alloys. Physical Review B, 2011, 84, .	3.2	49
39	The Atomic Site Occupancies in the Fe-Cr Ïƒ-Phase. Solid State Phenomena, 2011, 170, 13-16.	0.3	3
40	Influence of the Magnetic State on the Chemical Order-Disorder Transition Temperature in Fe-Ni Permalloy. Physical Review Letters, 2010, 105, 167208.	7.8	34
41	Comment on â€œThermal Signatures of the Kondo Volume Collapse in Ceriumâ€• Physical Review Letters, 2009, 102, 189601.	7.8	21
42	Stability in bcc Transition Metals: Madelung and Band-Energy Effects due to Alloying. Physical Review Letters, 2009, 103, 235501.	7.8	38
43	Surface segregation energies in low-index open surfaces of bimetallic transition metal alloys. Surface Science, 2009, 603, 91-96.	1.9	98
44	Thermodynamic reassessment of the Niâ€“Ru system and assessment of the Alâ€“Niâ€“Ru system at 1273â€“1523 K using ab initio calculations. Acta Materialia, 2008, 56, 4062-4069.	7.9	17
45	New generation of Ni-based superalloys designed on the basis of first-principles calculations. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2008, 497, 18-24.	5.6	38
46	Double-segregation effect in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Ag</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:msub><mml:mi mathvariant="normal">Pd</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow><mml:msub><mml:mi mathvariant="normal">Ru</mml:mi><mml:mrow><mml:mo>(</mml:mo><mml:mn>0001</mml:mn><mml:mo>)</mml:mo></mml:mrow> film nanostructures. Physical Review B, 2008, 77, .	3.2	24
47	New Pt-based Superalloy System Designed from First Principles. Materials Research Society Symposia Proceedings, 2008, 1128, 52801.	0.1	0
48	Magnetic state, magnetovolume effects, and atomic order in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Fe</mml:mi><mml:mn>65</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">Ni</mml:mi><mml:mn>35</mml:mn></mml:msub></mml:mrow></mml:math>Invar alloy: A first principles study. Physical Review B, 2007, 76, .	3.2	71
49	Magnetic exchange interactions in the paramagnetic state of hcp Gd. Journal of Physics Condensed Matter, 2007, 19, 326218.	1.8	24
50	Ab initio investigation of magnetic ordering and spin-glass transition in Cu-rich Cuâ€“Mn systems. Journal of Magnetism and Magnetic Materials, 2007, 310, 1561-1563.	2.3	0
51	Magnetism and origin of non-monotonous concentration dependence of the bulk modulus in Fe-rich alloys with Si, Ge and Sn: a first-principles study. Journal of Physics Condensed Matter, 2006, 18, 6677-6689.	1.8	25
52	Magnetic properties ofFeâ•Co(001)superlattices from first-principles theory. Physical Review B, 2006, 74, .	3.2	6
53	Ab initio calculations of elastic constants of the bcc Vâ€“Nb system at high pressures. Journal of Physics and Chemistry of Solids, 2006, 67, 2056-2064.	4.0	47
54	Fermi surface nesting and pre-martensitic softening in V and Nb at high pressures. Journal of Physics Condensed Matter, 2006, 18, 5079-5085.	1.8	69

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55	Electronic structure analysis of the pressure induced metamagnetic transition and magnetovolume anomaly in Fe3Câ€"cementite. Journal of Physics Condensed Matter, 2005, 17, 7345-7352.	1.8	11
56	Magnetic anisotropy ofL10FePt andFe1âˆ'xMnxPt. Physical Review B, 2005, 71, .	3.2	113
57	Surface energies and work functions of the transition metal carbides. Surface Science, 2004, 557, 243-254.	1.9	117
58	Adsorption and Dissociation of O2on Ptâˆ'Co and Ptâˆ'Fe Alloys. Journal of the American Chemical Society, 2004, 126, 4717-4725.	13.7	615
59	Pareto-optimal alloys. Applied Physics Letters, 2003, 83, 4527-4529.	3.3	43
60	Electronic structure calculations of Î´-Pu based alloys. Materials Research Society Symposia Proceedings, 2003, 802, 209.	0.1	0
61	Monte Carlo simulations of the stability of Â-Pu. Journal of Physics Condensed Matter, 2003, 15, L371-L376.	1.8	24
62	Theory for Î´-Pu and Î´-Pu Based Alloys. AIP Conference Proceedings, 2003, , .	0.4	0
63	Combined Electronic Structure and Evolutionary Search Approach to Materials Design. Physical Review Letters, 2002, 88, 255506.	7.8	248
64	Anode Materials for Low-Temperature Fuel Cells: A Density Functional Theory Study. Journal of Catalysis, 2001, 199, 123-131.	6.2	330
65	Constitutional and thermal point defects inB2NiAl. Physical Review B, 2000, 61, 6003-6018.	3.2	150
66	First-principles calculations of the vacancy formation energy in transition and noble metals. Physical Review B, 1999, 59, 11693-11703.	3.2	250
67	Surface segregation energies in transition-metal alloys. Physical Review B, 1999, 59, 15990-16000.	3.2	902
68	Calculated surface segregation in transition metal alloys. Computational Materials Science, 1999, 15, 119-143.	3.0	231
69	How a gold substrate can increase the reactivity of a Pt overlayer. Surface Science, 1999, 426, 395-409.	1.9	258
70	Development of Finnisâ€"Sinclair type potentials for Pb, Pbâ€"Bi, and Pbâ€"Ni systems: application to surface segregation. Acta Materialia, 1998, 46, 3027-3032.	7.9	30
71	Total energy calculations of random alloys: Supercell, Connolly-Williams, and CPA methods. Computational Materials Science, 1998, 10, 302-305.	3.0	17
72	Submonolayer growth of Pd on Cu(111) studied by scanning tunneling microscopy. Surface Science, 1998, 408, 43-56.	1.9	76

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73	The surface energy of metals. Surface Science, 1998, 411, 186-202.	1.9	2,342
74	Crystal-Structure Contribution to the Solid Solubility in Transition Metal Alloys. Physical Review Letters, 1998, 80, 1240-1243.	7.8	30
75	Heteroepitaxial subsurface growth mode resulting in interlayer mixing. Physical Review B, 1997, 55, 1380-1383.	3.2	61
76	Ab initio calculations of partial molar properties in the single-site approximation. Physical Review B, 1997, 55, 8801-8807.	3.2	26
77	Phase diagrams for surface alloys. Physical Review B, 1997, 56, 5822-5834.	3.2	391
78	Calculated site substitution in ternaryÎ³	IH-Ni3Al: Temperature and composition effects. Physical Review B, 1997, 55, 856-874.	3.2	138
79	Alloy Formation and Surface Segregation in Zeolite-Supported Ptâ^'Pd Bimetallic Catalysts. Journal of Physical Chemistry B, 1997, 101, 1861-1868.	2.6	68
80	Growth of Co on Cu(111): subsurface growth of trilayer Co islands. Surface Science, 1997, 387, 86-101.	1.9	106
81	Locally self-consistent Greenâ€™s function approach to the electronic structure problem. Physical Review B, 1997, 56, 9319-9334.	3.2	205
82	Surface electronic structure and reactivity of transition and noble metals1Communication presented at the First Francqui Colloquium, Brussels, 19â€“20 February 1996.1. Journal of Molecular Catalysis A, 1997, 115, 421-429.	4.8	1,166
83	Order-NGreen's Function Technique for Local Environment Effects in Alloys. Physical Review Letters, 1996, 76, 4203-4206.	7.8	210
84	Calculated site substitution in Î³â€²-Ni3Al. Solid State Communications, 1996, 99, 813-817.	1.9	35
85	Magnetically induced crystal structure and phase stability inFe1â^'cCoc. Physical Review B, 1996, 54, 3380-3384.	3.2	65
86	Calculated Phase Diagram for theÎ³â‡ŒÎ±Transition in Ce. Physical Review Letters, 1995, 74, 2335-2338.	7.8	121
87	Madelung energy for random metallic alloys in the coherent potential approximation. Physical Review B, 1995, 51, 5773-5780.	3.2	165
88	Ground-state properties of ordered, partially ordered, and random Cu-Au and Ni-Pt alloys. Physical Review B, 1995, 51, 12958-12968.	3.2	91
89	Calculated orientation dependence of surface segregations inPt50Ni50. Physical Review B, 1994, 50, 2039-2042.	3.2	58
90	Electronic structure, thermal, and elastic properties of Al-Li random alloys. Physical Review B, 1994, 49, 14229-14237.	3.2	53

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91	Fermi surfaces and electronic topological transitions in metallic solid solutions. Physics Reports, 1994, 249, 353-419.	25.6	72
92	Self-consistent electronic structure and segregation profiles of the Cu-Ni (001) random-alloy surface. Physical Review B, 1994, 49, 11383-11396.	3.2	61
93	Electronic structure, thermodynamic and thermal properties of Ni-Al disordered alloys from LMTO-CPA-DFT calculations. Journal of Physics Condensed Matter, 1993, 5, 1271-1290.	1.8	21
94	Ab initio calculations of the electronic topological transition in Liî—¸Mg alloys. Solid State Communications, 1992, 83, 867-870.	1.9	83
95	Fast LMTO-CPA method for electronic structure calculations of disordered alloys: application to Cu-Ni and Cu-Au systems. Physics Letters, Section A: General, Atomic and Solid State Physics, 1991, 154, 407-412.	2.1	40
96	Atomic distribution of alloying additions between sublattices in the intermetallic compounds Ni3Al and NiAl II: Microscopic calculations and X-ray diffraction analysis. Journal of the Less Common Metals, 1988, 141, 191-200.	0.8	29
97	Analysis of the Alloying System in Ni-Base Superalloys Based on <i>Ab Initio</i> Study of Impurity Segregation to Ni Grain Boundary. Advanced Materials Research, 0, 278, 192-197.	0.3	18
98	Order and Disorder in Ni-Pt Single Crystals. Solid State Phenomena, 0, 172-174, 593-601.	0.3	5
99	Dependence of Vacancy-Solute Interactions on Magnetic State in Dilute Iron-Based Alloys. Solid State Phenomena, 0, 172-174, 979-984.	0.3	3
100	<i>Ab Initio</i> Calculations of Kinetic Properties in ZrC and TiC Carbides. Solid State Phenomena, 0, 172-174, 990-995.	0.3	12
101	Effect of Magnetism on Short-Range Order Formation in Fe-Si and Fe-Al Alloys. Solid State Phenomena, 0, 172-174, 618-623.	0.3	12
102	<i>Ab Initio</i> Based O-O Investigation and the Snoek Relaxation in Nb-O. Solid State Phenomena, 0, 184, 63-68.	0.3	1