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	The surface energy of metals. Surface Science, 1998, 411, 186-202.	1.9	2,342
2	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
3	Surface segregation energies in transition-metal alloys. Physical Review B, 1999, 59, 15990-16000.	3.2	902
4	Adsorption and Dissociation of O2on Ptâˆ'Co and Ptâˆ'Fe Alloys. Journal of the American Chemical Society, 2004, 126, 4717-4725.	13.7	615
5	Phase diagrams for surface alloys. Physical Review B, 1997, 56, 5822-5834.	3.2	391
6	Anode Materials for Low-Temperature Fuel Cells: A Density Functional Theory Study. Journal of Catalysis, 2001, 199, 123-131.	6.2	330
7	How a gold substrate can increase the reactivity of a Pt overlayer. Surface Science, 1999, 426, 395-409.	1.9	258
8	First-principles calculations of the vacancy formation energy in transition and noble metals. Physical Review B, 1999, 59, 11693-11703.	3.2	250
9	Combined Electronic Structure and Evolutionary Search Approach to Materials Design. Physical Review Letters, 2002, 88, 255506.	7.8	248
10	Calculated surface segregation in transition metal alloys. Computational Materials Science, 1999, 15, 119-143.	3.0	231
11	Order-NGreen's Function Technique for Local Environment Effects in Alloys. Physical Review Letters, 1996, 76, 4203-4206.	7.8	210
12	Locally self-consistent Greenâ€™s function approach to the electronic structure problem. Physical Review B, 1997, 56, 9319-9334.	3.2	205
13	Madelung energy for random metallic alloys in the coherent potential approximation. Physical Review B, 1995, 51, 5773-5780.	3.2	165
14	Constitutional and thermal point defects inB2NiAl. Physical Review B, 2000, 61, 6003-6018.	3.2	150
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	Calculated site substitution in ternaryÎ³	IH-Ni3Al: Temperature and composition effects. Physical Review B, 1997, 55, 856-874.	3.2	138
17	Calculated Phase Diagram for theÎ³â‡ŒÎ±Transition in Ce. Physical Review Letters, 1995, 74, 2335-2338.	7.8	121
18	Surface energies and work functions of the transition metal carbides. Surface Science, 2004, 557, 243-254.	1.9	117

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19	Magnetic anisotropy ofL10FePt andFe1âˆ'xMnxPt. Physical Review B, 2005, 71, .	3.2	113
20	Growth of Co on Cu(111): subsurface growth of trilayer Co islands. Surface Science, 1997, 387, 86-101.	1.9	106
21	Surface segregation energies in low-index open surfaces of bimetallic transition metal alloys. Surface Science, 2009, 603, 91-96.	1.9	98
22	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
23	Long-ranged interactions in bcc NbMoTaW high-entropy alloys. Materials Research Letters, 2017, 5, 35-40.	8.7	86
24	Ab initio calculations of the electronic topological transition in Liî—¸Mg alloys. Solid State Communications, 1992, 83, 867-870.	1.9	83
25	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
26	Submonolayer growth of Pd on Cu(111) studied by scanning tunneling microscopy. Surface Science, 1998, 408, 43-56.	1.9	76
27	Fermi surfaces and electronic topological transitions in metallic solid solutions. Physics Reports, 1994, 249, 353-419.	25.6	72
28	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
29	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
30	Alloy Formation and Surface Segregation in Zeolite-Supported Ptâ˜'Pd Bimetallic Catalysts. Journal of Physical Chemistry B, 1997, 101, 1861-1868.	2.6	68
31	Magnetically induced crystal structure and phase stability inFe1âˆ'cCoc. Physical Review B, 1996, 54, 3380-3384.	3.2	65
32	Vacancyâ€“solute interactions in ferromagnetic and paramagnetic bcc iron: Ab initio calculations. Journal of Nuclear Materials, 2011, 419, 248-255.	2.7	63
33	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
34	Heteroepitaxial subsurface growth mode resulting in interlayer mixing. Physical Review B, 1997, 55, 1380-1383.	3.2	61
35	Temperature dependence of the stacking-fault Gibbs energy for Al, Cu, and Ni. Physical Review B, 2018, 98, .	3.2	61
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:n Alloy. Physical Review Letters, 2011, 107, 205504.	7.8	60

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37	Calculated orientation dependence of surface segregations inPt50Ni50. Physical Review B, 1994, 50, 2039-2042.	3.2	58
38	Importance of Correlation Effects in hcp Iron Revealed by a Pressure-Induced Electronic Topological Transition. Physical Review Letters, 2013, 110, 117206.	7.8	58
39	Electronic structure, thermal, and elastic properties of Al-Li random alloys. Physical Review B, 1994, 49, 14229-14237.	3.2	53
40	First-principles study of elastic properties of Cr- and Fe-rich Fe-Cr alloys. Physical Review B, 2011, 84, .	3.2	49
41	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
42	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
43	Pareto-optimal alloys. Applied Physics Letters, 2003, 83, 4527-4529.	3.3	43
44	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
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	Stability in bcc Transition Metals: Madelung and Band-Energy Effects due to Alloying. Physical Review Letters, 2009, 103, 235501.	7.8	38
47	First-principles study of interactions between substitutional solutes in bcc iron. Journal of Nuclear Materials, 2016, 475, 140-148.	2.7	37
48	Calculated site substitution in Î³â€²-Ni3Al. Solid State Communications, 1996, 99, 813-817.	1.9	35
49	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
50	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
51	Stacking-fault energy and anti-Invar effect in Fe-Mn alloy from first principles. Physical Review B, 2012, 86, .	3.2	33
52	Multi-length scale modeling of martensitic transformations in stainless steels. Acta Materialia, 2012, 60, 6508-6517.	7.9	31
53	Vacancy-cluster mechanism of metal-atom diffusion in substoichiometric carbides. Physical Review B, 2013, 87, .	3.2	31
54	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

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55	Crystal-Structure Contribution to the Solid Solubility in Transition Metal Alloys. Physical Review Letters, 1998, 80, 1240-1243.	7.8	30
56	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
57	First-principles study of point defects in Ni₃Al. Philosophical Magazine, 2014, 94, 20-34.	1.6	28
58	Ab initio calculations of partial molar properties in the single-site approximation. Physical Review B, 1997, 55, 8801-8807.	3.2	26
59	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
60	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
61	Monte Carlo simulations of the stability of Â-Pu. Journal of Physics Condensed Matter, 2003, 15, L371-L376.	1.8	24
62	Magnetic exchange interactions in the paramagnetic state of hcp Gd. Journal of Physics Condensed Matter, 2007, 19, 326218.	1.8	24
63	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: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></mml:msub></mml:mrow></mml:math> film nanostructures. Physical Review B, 2008, 77, .	3.2	24
64	Short-range order in face-centered cubic VCoNi alloys. Physical Review Materials, 2020, 4, .	2.4	24
65	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
66	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
67	Comment on â€œThermal Signatures of the Kondo Volume Collapse in Ceriumâ€• Physical Review Letters, 2009, 102, 189601.	7.8	21
68	Effective interactions and atomic ordering in Ni-rich Ni-Re alloys. Physical Review B, 2016, 94, .	3.2	19
69	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
70	Total energy calculations of random alloys: Supercell, Connolly-Williams, and CPA methods. Computational Materials Science, 1998, 10, 302-305.	3.0	17
71	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
72	Direct atom probe tomography observations of concentration fluctuations in Feâ€“Cr solid solution. Scripta Materialia, 2015, 98, 13-15.	5.2	17

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73	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
74	Configurational thermodynamics of the Fe-CrÏƒ phase. Physical Review B, 2011, 84, .	3.2	16
75	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
76	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
77	<i>Ab Initio</i> Calculations of Kinetic Properties in ZrC and TiC Carbides. Solid State Phenomena, 0, 172-174, 990-995.	0.3	12
78	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
79	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
80	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
81	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
82	Ab initio surface free energies of tungsten with full account of thermal excitations. Physical Review B, 2022, 105, .	3.2	10
83	Ab initio simulations of the surface free energy of TiN(001). Physical Review B, 2021, 103, .	3.2	9
84	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
85	Magnetic properties ofFeâ•Co(001)superlattices from first-principles theory. Physical Review B, 2006, 74, .	3.2	6
86	Order and Disorder in Ni-Pt Single Crystals. Solid State Phenomena, 0, 172-174, 593-601.	0.3	5
87	Evidence for the antiferromagnetic ground state of Zr2TiAl: a first-principles study. Journal of Physics Condensed Matter, 2017, 29, 265801.	1.8	5
88	Stability and ordering of bcc and hcp TiAl+Mo phases: An ab initio study. Computational Materials Science, 2022, 205, 111163.	3.0	5
89	Single-site mean-field approach to thermal defects in binary ordered alloys. Philosophical Magazine, 2014, 94, 1192-1201.	1.6	4
90	Towards predictive simulations of spinodal decomposition in Fe-Cr alloys. Computational Materials Science, 2022, 202, 110955.	3.0	4

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91	Solubility and segregation of B in paramagnetic fcc Fe. Physical Review Materials, 2022, 6, .	2.4	4
92	The Atomic Site Occupancies in the Fe-Cr Ïƒ-Phase. Solid State Phenomena, 2011, 170, 13-16.	0.3	3
93	Dependence of Vacancy-Solute Interactions on Magnetic State in Dilute Iron-Based Alloys. Solid State Phenomena, 0, 172-174, 979-984.	0.3	3
94	Ab Initio Study of Advanced Metallic Nuclear Fuels for Fast Breeder Reactors. Materials Research Society Symposia Proceedings, 2012, 1444, 67.	0.1	3
95	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
96	<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
97	Structural vacancies in (Ti,Al)N: An ab initio study. Physical Review Materials, 2022, 6, .	2.4	1
98	Electronic structure calculations of Î´-Pu based alloys. Materials Research Society Symposia Proceedings, 2003, 802, 209.	0.1	0
99	Theory for Î´-Pu and Î´-Pu Based Alloys. AIP Conference Proceedings, 2003, , .	0.4	0
100	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
101	New Pt-based Superalloy System Designed from First Principles. Materials Research Society Symposia Proceedings, 2008, 1128, 52801.	0.1	0
102	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