Igor A Abrikosov

List of Publications by Year
in descending order

199	10,358	31976	38395
papers	citations	53 h-index	95 g-index

202	202	202	9055
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Anisotropic Lattice Distortions in Random Alloys from First-Principles Theory. Physical Review Letters, 2001, 87, 156401.	7.8	556
2	Origin of the Invar effect in ironâ€“nickel alloys. Nature, 1999, 400, 46-49.	27.8	487
3	Lattice dynamics of anharmonic solids from first principles. Physical Review B, 2011, 84, .	3.2	482
4	Temperature dependent effective potential method for accurate free energy calculations of solids. Physical Review B, 2013, 87, .	3.2	397
5	Modeling ofCeO2,Ce2O3, andCeO2â˜’xin theLDA+Uformalism. Physical Review B, 2007, 75, .	3.2	333
6	Phonon related properties of transition metals, their carbides, and nitrides: A first-principles study. Journal of Applied Physics, 2007, 101, 123519.	2.5	312
7	Temperature-dependent effective third-order interatomic force constants from first principles. Physical Review B, 2013, 88, .	3.2	266
8	Configurational thermodynamics of alloys from first principles: effective cluster interactions. Reports on Progress in Physics, 2008, 71, 046501.	20.1	264
9	Order-NGreen's Function Technique for Local Environment Effects in Alloys. Physical Review Letters, 1996, 76, 4203-4206.	7.8	210
10	Mixing and decomposition thermodynamics ofcâ˜’Ti1â˜’xAlxNfrom first-principles calculations. Physical Review B, 2007, 75, .	3.2	198
11	Electronic origin of the anomalous stability of Fe-rich bcc Fe-Cr alloys. Physical Review B, 2006, 73, .	3.2	175
12	The most incompressible metal osmium at static pressures above 750 gigapascals. Nature, 2015, 525, 226-229.	27.8	159
13	Fe-N system at high pressure reveals a compound featuring polymeric nitrogen chains. Nature Communications, 2018, 9, 2756.	12.8	153
14	Electrically and Mechanically Tunable Electron Spins in Silicon Carbide Color Centers. Physical Review Letters, 2014, 112, 187601.	7.8	152
15	Magnetic Self-Organized Atomic Laminate from First Principles and Thin Film Synthesis. Physical Review Letters, 2013, 110, 195502.	7.8	146
16	Calculated magnetic properties of binary alloys between Fe, Co, Ni, and Cu. Physical Review B, 1999, 59, 419-430.	3.2	143
17	Synthesis of Ti3AuC2, Ti3Au2C2 and Ti3IrC2 by noble metal substitution reaction in Ti3SiC2 for high-temperature-stable Ohmic contacts to SiC. Nature Materials, 2017, 16, 814-818.	27.5	142
18	Effect of magnetic disorder and strong electron correlations on the thermodynamics of CrN. Physical Review B, 2010, 82, .	3.2	129

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19	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>0.5</mml:mn></mml:mrow></mml:msub></mml:math>Al<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>0.5</mml:mn></mml:mrow></mml:msub></mml:math>N alloys: Dependence of elastic constants on size and shape of the supercell model and their convergence. Physical Review B, 2	3.2	125
20	Thermochromic Leadâ€Free Halide Double Perovskites. Advanced Functional Materials, 2019, 29, 1807375.	14.9	120
21	Competition between magnetic structures in the Fe rich fcc FeNi alloys. Physical Review B, 2007, 76, .	3.2	119
22	Cerium oxide nanoparticles with antioxidant capabilities and gadolinium integration for MRI contrast enhancement. Scientific Reports, 2018, 8, 6999.	3.3	111
23	Significant elastic anisotropy in Ti1â^'xAlxN alloys. Applied Physics Letters, 2010, 97, .	3.3	107
24	Valence-Band Hybridization and Core Level Shifts in Random Ag-Pd Alloys. Physical Review Letters, 2001, 87, 176403.	7.8	101
25	Pressure and temperature dependence of the zero-field splitting in the ground state of NV centers in diamond: A first-principles study. Physical Review B, 2014, 90, .	3.2	97
26	Improving thermal stability of hard coating films via a concept of multicomponent alloying. Applied Physics Letters, 2011, 99, .	3.3	95
27	On the interaction of toxic Heavy Metals (Cd, Hg, Pb) with graphene quantum dots and infinite graphene. Scientific Reports, 2017, 7, 3934.	3.3	94
28	Anharmonicity and Ultralow Thermal Conductivity in Lead-Free Halide Double Perovskites. Physical Review Letters, 2020, 125, 045701.	7.8	90
29	High-Pressure Synthesis of Dirac Materials: Layered van der Waals Bonded <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow><mml:mi>BeN</mml:mi></mml:mrow><mml:mrow><mml:mn>4</mml:mn></mml:mrow> Polymorph. Physical Review Letters, 2021, 126, 175501.	7.8	90
30	Anomalously enhanced superconductivity andab initiolattice dynamics in transition metal carbides and nitrides. Physical Review B, 2005, 72, .	3.2	84
31	Phase Stability and Elasticity of TiAlN. Materials, 2011, 4, 1599-1618.	2.9	80
32	Leadâ€Free Halide Double Perovskite Cs₂AgBiBr₆ with Decreased Band Gap. Angewandte Chemie - International Edition, 2020, 59, 15191-15194.	13.8	80
33	Pressure-Induced Invar Effect in Fe-Ni Alloys. Physical Review Letters, 2001, 86, 4851-4854.	7.8	78
34	Temperature dependence of TiN elastic constants fromab initiomolecular dynamics simulations. Physical Review B, 2013, 87, .	3.2	78
35	Modeling the actinides with disordered local moments. Physical Review B, 2003, 67, .	3.2	74
36	Identification of Si-vacancy related room-temperature qubits in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>4</mml:mn><mml:mi>H</mml:mi> silicon carbide. Physical Review B, 2017, 96, .	3.2	74

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37	Origin of magnetic frustrations inFeâ^'NiInvar alloys. Physical Review B, 2005, 71, .	3.2	73
38	Equation of state of paramagnetic CrN fromab initiomolecular dynamics. Physical Review B, 2012, 85, .	3.2	70
39	Highâ€Pressure Synthesis of a Nitrogenâ€Rich Inclusion Compound ReN₈â‹…xâ€‰N₂ with Conjugated Polymeric Nitrogen Chains. Angewandte Chemie - International Edition, 2018, 57, 9048-9053.	13.8	70
40	Pressure enhancement of the isostructural cubic decomposition in Ti1â^'xAlxN. Applied Physics Letters, 2009, 95, .	3.3	67
41	Dirac points with giant spin-orbit splitting in the electronic structure of two-dimensional transition-metal carbides. Physical Review B, 2015, 92, .	3.2	65
42	High-pressure synthesis of ultraincompressible hard rhenium nitride pernitride Re2(N2)(N)2 stable at ambient conditions. Nature Communications, 2019, 10, 2994.	12.8	65
43	Magnetic and electronic structure of(Ga1â^'xMnx)As. Physical Review B, 2003, 67, .	3.2	64
44	Assessing the SCAN functional for itinerant electron ferromagnets. Physical Review B, 2018, 98, .	3.2	64
45	Theoretical study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Ce</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>doped with tetravalent ions. Physical Review B, 2007, 76, .	3.2	61
46	Lattice Vibrations Change the Solid Solubility of an Alloy at High Temperatures. Physical Review Letters, 2016, 117, 205502.	7.8	60
47	Wave function extended Lagrangian Born-Oppenheimer molecular dynamics. Physical Review B, 2010, 82, .	3.2	59
48	Theoretical model of dynamic spin polarization of nuclei coupled to paramagnetic point defects in diamond and silicon carbide. Physical Review B, 2015, 92, .	3.2	59
49	First-principles solution to the problem of Mo lattice stability. Physical Review B, 2008, 77, .	3.2	58
50	Importance of Correlation Effects in hcp Iron Revealed by a Pressure-Induced Electronic Topological Transition. Physical Review Letters, 2013, 110, 117206.	7.8	58
51	Structural and magnetic ground-state properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î³</mml:mi></mml:math>-FeMn alloys fromab initiocalculations. Physical Review B, 2011, 84, .	3.2	56
52	First principles calculation of spin-related quantities for point defect qubit research. Npj Computational Materials, 2018, 4, .	8.7	56
53	Nearâ€Infrared Lightâ€Responsive Cuâ€Doped Cs₂AgBiBr₆. Advanced Functional Materials, 2020, 30, 2005521.	14.9	56
54	Realization of an Ideal Cairo Tessellation in Nickel Diazenide NiN₂: High-Pressure Route to Pentagonal 2D Materials. ACS Nano, 2021, 15, 13539-13546.	14.6	55

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55	Site preference and effect of alloying on elastic properties of ternary<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>B</mml:mi></mml:math>2 NiAl-based alloys. Physical Review B, 2012, 85, .	3.2	53
56	Nitrogen vacancy, self-interstitial diffusion, and Frenkel-pair formation/dissociation in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>B</mml:mi><mml:mn>1</mml:mn></mml:mrow></mml:m studied byab initioand classical molecular dynamics with optimized potentials. Physical Review B, 2015, 91, .	3.2	53
57	Impact of electronic correlations on the equation of state and transport in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Îµ</mml:mi></mml:math>-Fe. Physical Review B, 2014, 90, .	3.2	50
58	Spin and photophysics of carbon-antisite vacancy defect in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>4</mml:mn><mml:mi>H</mml:mi></mml:mrow></mml: carbide: A potential quantum bit. Physical Review B, 2015, 91, .	3.2	50
59	Core-level shifts in fcc random alloys: A first-principles approach. Physical Review B, 2005, 72, .	3.2	49
60	First-principles study of dislocations in hcp metals through the investigation of the (<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 5 twin boundary. Physical Review B, 2011, 84, .	3.2	49
61	Magnetic collapse and the behavior of transition metal oxides at high pressure. Physical Review B, 2016, 94, .	3.2	47
62	First-principles study of the effect of nitrogen vacancies on the decomposition pattern in cubic Ti1âˆ’xAlxN1âˆ’y. Applied Physics Letters, 2008, 92, .	3.3	46
63	Vibrational free energy and phase stability of paramagnetic and antiferromagnetic CrN fromab initiomolecular dynamics. Physical Review B, 2014, 89, .	3.2	46
64	Theoretical unification of hybrid-DFT and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mtext>DFT</mml:mtext><mml:mo>â€‰</mml:mo> for the treatment of localized orbitals. Physical Review B, 2014, 90, .	3.2	46
65	Temperature-dependent elastic properties of Ti1âˆ’xAlxN alloys. Applied Physics Letters, 2015, 107, .	3.3	46
66	Role of stoichiometric and nonstoichiometric defects on the magnetic properties of the half-metallic ferromagnet NiMnSb. Physical Review B, 2006, 73, .	3.2	45
67	Magnetically driven anisotropic structural changes in the atomic laminate<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>2</mml:mn></mml:msub><mml:mi>GaC</mml:mi></mml:mrow></mml:math>. Physical Review B, 2016, 93, .	3.2	44
68	Structural and electronic properties of Li-intercalated graphene on SiC(0001). Physical Review B, 2016, 93, .	3.2	44
69	Systematic ab initio investigation of the elastic modulus in quaternary transition metal nitride alloys and their coherent multilayers. Acta Materialia, 2017, 127, 124-132.	7.9	44
70	Strong impact of lattice vibrations on electronic and magnetic properties of paramagnetic Fe revealed by disordered local moments molecular dynamics. Physical Review B, 2016, 93, .	3.2	43
71	Core-level shifts in complex metallic systems from first principle. Physica Status Solidi (B): Basic Research, 2006, 243, 2447-2464.	1.5	42
72	Electronic properties and magnetism of iron at the Earth's inner core conditions. Physical Review B, 2013, 87, .	3.2	42

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73	Stabilization of point-defect spin qubits by quantum wells. Nature Communications, 2019, 10, 5607.	12.8	42
74	Large piezoelectric response of quarternary wurtzite nitride alloys and its physical origin from first principles. Physical Review B, 2015, 92, .	3.2	41
75	Stability of the Anomalous Large-Void CoSn Structure. Physical Review Letters, 1997, 79, 1333-1336.	7.8	39
76	First principles predictions of magneto-optical data for semiconductor point defect identification: the case of divacancy defects in 4Hâ€“SiC. New Journal of Physics, 2018, 20, 023035.	2.9	39
77	Metastable silica high pressure polymorphs as structural proxies of deep Earth silicate melts. Nature Communications, 2018, 9, 4789.	12.8	39
78	Unified cluster expansion method applied to the configurational thermodynamics of cubic Ti<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub><mml:mrow	3.2	38
79	xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mi>x</mml:mi></mml:mrow Ab initiocalculation of the solution enthalpies of substitutional and interstitial impurities in paramagnetic fcc Fe. Physical Review B, 2014, 90, .	3.2	38
80	Electronâ€“electron scattering and thermal conductivity ofÏµ-iron at Earthâ€™s core conditions. New Journal of Physics, 2017, 19, 073022.	2.9	38
81	Numerical investigation of the validity of the Slater-Janak transition-state model in metallic systems. Physical Review B, 2005, 72, .	3.2	36
82	Surface segregation energy in bcc Fe-rich Fe-Cr alloys. Physical Review B, 2007, 75, .	3.2	36
83	Highâ€Pressure Synthesis of Metalâ€“Inorganic Frameworks Hf 4 N 20 â‹…N 2 , WN 8 â‹…N 2 , and Os 5 N 28 â‹…3â€‰N 2 with Polymeric Nitrogen Linkers. Angewandte Chemie - International Edition, 2020, 59, 10321-10326.	13.8	36
84	Role of screening in the density functional applied to transition-metal defects in semiconductors. Physical Review B, 2013, 87, .	3.2	35
85	Materials synthesis at terapascal static pressures. Nature, 2022, 605, 274-278.	27.8	35
86	Bulk ordering and surface segregation inNi50Pt50. Physical Review B, 2001, 64, .	3.2	34
87	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
88	High pressure and high temperature stabilization of cubic AlN in Ti0.60Al0.40N. Journal of Applied Physics, 2013, 113, .	2.5	34
89	Leadâ€Free Halide Double Perovskite Cs₂AgBiBr₆ with Decreased Band Gap. Angewandte Chemie, 2020, 132, 15303-15306.	2.0	34
90	Fully relativistic spin-polarized exact muffin-tin-orbital method. Physical Review B, 2005, 71, .	3.2	33

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91	Multiple Ï€-bands and Bernal stacking of multilayer graphene on C-face SiC, revealed by nano-Angle Resolved Photoemission. Scientific Reports, 2014, 4, 4157.	3.3	33
92	Pressure-Induced Site-Selective Mott Insulator-Metal Transition in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Fe</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml: Physical Review X, 2018, 8, .	8.9	32
93	Role of N defects in paramagnetic CrN at finite temperatures from first principles. Physical Review B, 2015, 91, .	3.2	30
94	Electronic structure investigation of the cubic inverse perovskite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Sc</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub> Physical Review B, 2008, 78, .	3.2	29
95	Charge neutrality in epitaxial graphene on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>6</mml:mn><mml:mi>H</mml:mi> via nitrogen intercalation. Physical Review B, 2015, 92, .	3.2	29
96	Stabilization of Polynitrogen Anions in Tantalumâ€“Nitrogen Compounds at High Pressure. Angewandte Chemie - International Edition, 2021, 60, 9003-9008.	13.8	29
97	Metastability of fcc-related Si-N phases. Physical Review B, 2008, 78, .	3.2	28
98	Single-monolayer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SiN</mml:mtext></mml:mrow><mml:mi>x</mml:mi> in TiN: A first-principles study. Physical Review B, 2010, 81, .	3.2	28
99	Strong electron correlations stabilize paramagnetic cubic Cr1â^'xAlxN solid solutions. Applied Physics Letters, 2013, 102, .	3.3	28
100	Superioniclike Diffusion in an Elemental Crystal: bcc Titanium. Physical Review Letters, 2019, 123, 105501.	7.8	28
101	Identification of divacancy and silicon vacancy qubits in 6H-SiC. Applied Physics Letters, 2019, 114, 112107.	3.3	28
102	Core-level shifts for two- and three-dimensional bimetallicPdxCu1â^'xandPdxAg1â^'xalloys on Ru(0001). Physical Review B, 2005, 72, .	3.2	27
103	Significant configurational dependence of the electromechanical coupling constant of B0.125Al0.875N. Applied Physics Letters, 2009, 94, .	3.3	26
104	Ab initiostudy of disorder broadening of core photoemission spectra in randomCuâ^'PdandAgâ^'Pdalloys. Physical Review B, 2005, 72, .	3.2	25
105	Ab initiolattice stability of fcc and hcp Feâ€“Mn random alloys. Journal of Physics Condensed Matter, 2010, 22, 295402.	1.8	25
106	Including the effects of pressure and stress in thermodynamic functions. Physica Status Solidi (B): Basic Research, 2014, 251, 81-96.	1.5	25
107	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: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
108	Effect of dispersion corrections on ab initio predictions of graphite and diamond properties under pressure. Physical Review B, 2018, 98, .	3.2	24

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109	Exchange interactions in paramagnetic amorphous and disordered crystalline<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>CrN</mml:mi></mml:math>-based systems. Physical Review B, 2013, 88, .	3.2	23
110	Emergence of quantum critical charge and spin-state fluctuations near the pressure-induced Mott transition in MnO, FeO, CoO, and NiO. Physical Review B, 2020, 101, .	3.2	21
111	Revealing the Complex Nature of Bonding in the Binary High-Pressure Compound <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>FeO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn> Physical Review Letters, 2021, 126, 106001.	7.8	21
112	Ab initio calculations of elastic properties of Ru1âˆ’xNixAl superalloys. Applied Physics Letters, 2009, 94, .	3.3	20
113	Effect of pressure on phase stability in Fe-Cr alloys. Physical Review B, 2011, 84, .	3.2	20
114	First-principles calculations of properties of orthorhombic iron carbide<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Fe</mml:mi><mml:mn>7</mml:mn></mml: mathvariant="normal">C</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>at the Earth's core conditions. Physical Review B, 2015, 91, .	3.2	20
115	Impact of anharmonic effects on the phase stability, thermal transport, and electronic properties of AlN. Physical Review B, 2016, 94, .	3.2	20
116	Penta- and hexa-coordinated beryllium and phosphorus in high-pressure modifications of CaBe2P2O8. Nature Communications, 2019, 10, 2800.	12.8	20
117	Elinvar effect in Î²-Ti simulated by on-the-fly trained moment tensor potential. New Journal of Physics, 2020, 22, 113005.	2.9	20
118	Effect of thermal expansion, electronic excitations, and disorder on the Curie temperature of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ni</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</mml:mn> Physical Review B, 2009, 79, .	3.2	19
119	Elastic properties of fcc Fe-Mn-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>X</mml:mi></mml:math>(<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 347 Td (xmlns:mml="ht	3.2	19
120	Stability of the ternary perovskites<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Sc</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub> xmlns:mml="http://www.w3.org/1998/Math/MathML"		

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127	Ordered Phases inCu2NiZn: A First-Principles Monte Carlo Study. Physical Review Letters, 1998, 81, 188-191.	7.8	15
128	Magnetic interactions in NiO at ultrahigh pressure. Physical Review B, 2016, 93, .	3.2	15
129	Energy dependence of exact muffin-tin-orbital structure constants. Physical Review B, 2007, 75, .	3.2	14
130	Experimental and theoretical evidence of charge transfer in multi-component alloys â€“ how chemical interactions reduce atomic size mismatch. Materials Chemistry Frontiers, 2021, 5, 5746-5759.	5.9	14
131	Atomistic description of self-diffusion in molybdenum: A comparative theoretical study of non-Arrhenius behavior. Physical Review Materials, 2020, 4, .	2.4	14
132	Absence of a pressure-induced structural phase transition inTi3Alup to 25 GPa. Physical Review B, 2000, 63, .	3.2	13
133	Origin of the asymmetric spinodal decomposition in the Al-Zn system. Physical Review B, 2001, 64, .	3.2	13
134	Application of the Monte Carlo method to the problem of surface segregation simulation. JETP Letters, 2001, 73, 415-419.	1.4	13
135	Impact of lattice vibrations on equation of state of the hardest boron phase. Physical Review B, 2011, 83, .	3.2	13
136	High temperature phase decomposition in TixZryAlzN. AIP Advances, 2014, 4, .	1.3	13
137	Pressure-induced crossing of the core levels in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>5</mml:mn><mml:mi>d</mml:mi><mml:mrow></mml:mrow></mml:mrow></mml:math> Physical Review B, 2016, 93, .	3.2	13
138	Non-equilibrium vacancy formation energies in metastable alloys â€” A case study ofÂTi0.5Al0.5N. Materials and Design, 2017, 114, 484-493.	7.0	13
139	Magnetic and structural properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>FeC</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> at high pressures. Physical Review B, 2017, 96, .	3.2	13
140	Origin of the core-level binding energy shifts in Au nanoclusters. Physical Review B, 2017, 95, .	3.2	13
141	Suppression of disorder broadening of core-level photoelectron lines in CuAu alloys by inhomogeneous lattice distortion. Physical Review B, 2009, 79, .	3.2	12
142	Electronic correlations in Fe at Earth's inner core conditions: Effects of alloying with Ni. Physical Review B, 2015, 91, .	3.2	12
143	Nanodomain structure of single crystalline nickel oxide. Scientific Reports, 2021, 11, 3496.	3.3	12
144	Efficient and accurate determination of lattice-vacancy diffusion coefficients via non equilibriumab initiomolecular dynamics. Physical Review B, 2016, 93, .	3.2	11

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145	Charge disproportionation and site-selective local magnetic moments in the post-perovskite-type Fe2O3 under ultra-high pressures. Npj Computational Materials, 2019, 5, .	8.7	11
146	Temperature dependence of the Kohn anomaly in bcc Nb from first-principles self-consistent phonon calculations. Physical Review B, 2020, 101, .	3.2	11
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