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	Predicting elastic properties of hard-coating alloys using ab-initio and machine learning methods. Npj Computational Materials, 2022, 8, .	8.7	16
2	Correlation strength, orbital-selective incoherence, and local moments formation in the magnetic MAX-phase<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Mn</mml:mi><mml:mn>2</mml:mn></mml: Physical Review B, 2022, 105, .	3.2	3
3	Materials synthesis at terapascal static pressures. Nature, 2022, 605, 274-278.	27.8	35
4	Electronic and optical properties of crystalline nitrogen versus black phosphorus: A comparative first-principles study. Physical Review B, 2022, 105, .	3.2	3
5	Anionic N₁₈ Macrocycles and a Polynitrogen Double Helix in Novel Yttrium Polynitrides YN₆ and Y₂N₁₁ at 100â€…GPa. Angewandte Chemie - International Edition, 2022, 61, .	13.8	10
6	Local atomic configuration approach to the nonmonotonic concentration dependence of magnetic properties of Ni<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.svg"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Mn<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si3.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>+</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>Z<mml:ma	5.2	3
7	Photoluminescence at the ground-state level anticrossing of the nitrogen-vacancy center in diamond: A comprehensive study. Physical Review B, 2021, 103, .	3.2	16
8	Nanodomain structure of single crystalline nickel oxide. Scientific Reports, 2021, 11, 3496.	3.3	12
9	Modelling the thermodynamic data for hcp Zn and Cuâ€“Zn alloysâ€“ an ab initio and calphad approach. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2021, 72, 102253.	1.6	8
10	Stabilization of Polynitrogen Anions in Tantalumâ€“Nitrogen Compounds at High Pressure. Angewandte Chemie - International Edition, 2021, 60, 9003-9008.	13.8	29
11	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><mml: Physical Review Letters, 2021, 126, 106001.	7.8	21
12	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
13	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
14	Efficient prediction of elastic properties of Ti0.5Al0.5N at elevated temperature using machine learning interatomic potential. Thin Solid Films, 2021, 737, 138927.	1.8	4
15	Accurate prediction of high-temperature elastic constants of Ti0.5Al0.5N random alloy. Thin Solid Films, 2021, 735, 138872.	1.8	4
16	ADAQ: Automatic workflows for magneto-optical properties of point defects in semiconductors. Computer Physics Communications, 2021, 269, 108091.	7.5	8
17	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
18	Machine learning prediction of thermodynamic and mechanical properties of multicomponent Fe-Cr-based alloys. Physical Review Materials, 2021, 5, .	2.4	4

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19	Thermodynamic and electronic properties of ReN2 polymorphs at high pressure. Physical Review B, 2021, 104, .	3.2	1
20	Dipolar spin relaxation of divacancy qubits in silicon carbide. Npj Computational Materials, 2021, 7, .	8.7	7
21	Anharmonicity and Ultralow Thermal Conductivity in Lead-Free Halide Double Perovskites. Physical Review Letters, 2020, 125, 045701.	7.8	90
22	Achieving low elastic moduli of bcc Tiâ€“V alloys in vicinity of mechanical instability. AIP Advances, 2020, 10, 105322.	1.3	3
23	Nearâ€Infrared Lightâ€Responsive Cuâ€Doped Cs₂AgBiBr₆. Advanced Functional Materials, 2020, 30, 2005521.	14.9	56
24	Leadâ€Free Halide Double Perovskite Cs₂AgBiBr₆ with Decreased Band Gap. Angewandte Chemie - International Edition, 2020, 59, 15191-15194.	13.8	80
25	Leadâ€Free Halide Double Perovskite Cs₂AgBiBr₆ with Decreased Band Gap. Angewandte Chemie, 2020, 132, 15303-15306.	2.0	34
26	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
27	Temperature dependence of the Kohn anomaly in bcc Nb from first-principles self-consistent phonon calculations. Physical Review B, 2020, 101, .	3.2	11
28	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
29	Highâ€Pressure Synthesis of Metalâ€“Inorganic Frameworks Hf₄N₂₀â‹…N₂, WN₈â‹…N₂, and Os₅N₂₈â‹…3â€‰N₂ with Polymeric Nitrogen Linkers. Angewandte Chemie, 2020, 132, 10407-10412.	2.0	8
30	InnenrÃ¼cktitelbild: Highâ€Pressure Synthesis of Metalâ€“Inorganic Frameworks Hf₄N₂₀â‹…N₂, WN₈â‹…N₂, and Os₅N₂₈â‹…3â€‰N₂ with Polymeric Nitrogen Linkers (Angew. Chem.) Tj ETQq0 0 0 rgBT /Overlo	2.0	0
31	Temperature-dependent lattice dynamics of antiferromagnetic and ferromagnetic phases of FeRh. Physical Review B, 2020, 101, .	3.2	11
32	Elinvar effect in Î²-Ti simulated by on-the-fly trained moment tensor potential. New Journal of Physics, 2020, 22, 113005.	2.9	20
33	Atomistic description of self-diffusion in molybdenum: A comparative theoretical study of non-Arrhenius behavior. Physical Review Materials, 2020, 4, .	2.4	14
34	Theoretical modeling of interstitial carbon impurities in paramagnetic Fe-Mn alloys. Physical Review Materials, 2020, 4, .	2.4	3
35	Theoretical description of thermodynamic and mechanical properties of multicomponent bcc Fe-Cr-based alloys. Physical Review Materials, 2020, 4, .	2.4	2
36	Interstitial carbon in bcc HfNbTiVZr high-entropy alloy from first principles. Physical Review Materials, 2020, 4, .	2.4	4

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37	Design of Materials for Nuclear Energy Applications: First-Principles Calculations and Artificial Intelligence Methods. High Temperature, 2020, 58, 907-937.	1.0	3
38	The magnetization profile induced by the double magnetic proximity effect in an Fe/Fe0.30V0.70 superlattice. Applied Physics Letters, 2019, 115, .	3.3	2
39	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
40	Phase stability and electronic structure of iridium metal at the megabar range. Scientific Reports, 2019, 9, 8940.	3.3	17
41	Superionic‐like Diffusion in an Elemental Crystal: bcc Titanium. Physical Review Letters, 2019, 123, 105501.	7.8	28
42	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
43	Thermochromic Lead‐Free Halide Double Perovskites. Advanced Functional Materials, 2019, 29, 1807375.	14.9	120
44	Inverse pressure-induced Mott transition in TiPO4. Physical Review B, 2019, 99, .	3.2	2
45	High Pressure Investigation of the S–N₂ System up to the Megabar Range: Synthesis and Characterization of the SN₂ Solid. Inorganic Chemistry, 2019, 58, 9195-9204.	4.0	17
46	Penta- and hexa-coordinated beryllium and phosphorus in high-pressure modifications of CaBe2P2O8. Nature Communications, 2019, 10, 2800.	12.8	20
47	Identification of divacancy and silicon vacancy qubits in 6H-SiC. Applied Physics Letters, 2019, 114, 112107.	3.3	28
48	Stabilization of point-defect spin qubits by quantum wells. Nature Communications, 2019, 10, 5607.	12.8	42
49	Correlation between Ethylene Adsorption Energies and Core-Level Shifts for Pd Nanoclusters. Journal of Physical Chemistry C, 2019, 123, 2544-2548.	3.1	3
50	Effect of the lattice dynamics on the electronic structure of paramagnetic NiO within the disordered local moment picture. Physical Review B, 2018, 97, .	3.2	6
51	First principles predictions of magneto-optical data for semiconductor point defect identification: the case of divacancy defects in 4H–SiC. New Journal of Physics, 2018, 20, 023035.	2.9	39
52	Effect of dispersion corrections on ab initio predictions of graphite and diamond properties under pressure. Physical Review B, 2018, 98, .	3.2	24
53	Metastable silica high pressure polymorphs as structural proxies of deep Earth silicate melts. Nature Communications, 2018, 9, 4789.	12.8	39
54	First principles calculation of spin-related quantities for point defect qubit research. Npj Computational Materials, 2018, 4, .	8.7	56

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55	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:mrow><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review X, 2018, 8, .	8.9	82
56	Assessing the SCAN functional for itinerant electron ferromagnets. Physical Review B, 2018, 98, .	3.2	64
57	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
58	Fe-N system at high pressure reveals a compound featuring polymeric nitrogen chains. Nature Communications, 2018, 9, 2756.	12.8	153
59	Cerium oxide nanoparticles with antioxidant capabilities and gadolinium integration for MRI contrast enhancement. Scientific Reports, 2018, 8, 6999.	3.3	111
60	Resolving the debated atomic structure of the metastable cubic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Si</mml:mi><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mi>x</mml:mi></mml:msub></mml:mrow></mml:math> tissue phase in nanocomposites with TiN. Physical Review Materials, 2018, 2, .	2.4	0
61	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
62	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
63	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
64	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
65	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
66	Origin of the core-level binding energy shifts in Au nanoclusters. Physical Review B, 2017, 95, .	3.2	13
67	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></mml:mrow></mml:math> silicon carbide. Physical Review B, 2017, 96, .	3.2	74
68	Electronâ€“electron scattering and thermal conductivity ofÏµ-iron at Earthâ€™s core conditions. New Journal of Physics, 2017, 19, 073022.	2.9	38
69	Energyâ€surfaces from the upper bound of the Pauli kinetic energy. International Journal of Quantum Chemistry, 2016, 116, 1337-1341.	2.0	5
70	Impact of anharmonic effects on the phase stability, thermal transport, and electronic properties of AlN. Physical Review B, 2016, 94, .	3.2	20
71	Highly Efficient Free Energy Calculations of the Fe Equation of State Using Temperature-Dependent Effective Potential Method. Journal of Physical Chemistry A, 2016, 120, 8761-8768.	2.5	6
72	Finite-temperature elastic constants of paramagnetic materials within the disordered local moment picture fromab initiomolecular dynamics calculations. Physical Review B, 2016, 94, .	3.2	10

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73	High-Fidelity Bidirectional Nuclear Qubit Initialization in SiC. Physical Review Letters, 2016, 117, 220503.	7.8	16
74	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
75	Efficient and accurate determination of lattice-vacancy diffusion coefficients via non equilibriumab initiomolecular dynamics. Physical Review B, 2016, 93, .	3.2	11
76	Coherency effects on the mixing thermodynamics of cubic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ti</mml:mi><mml:mrow><mml:mn>1</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mo>/</mml:mo><mml:mi>TiN</mml:mi></mml:mrow></mml:math>(001) multilayers. Physical Review B, 2016, 93, .	3.2	10
77	Structural and electronic properties of Li-intercalated graphene on SiC(0001). Physical Review B, 2016, 93, .	3.2	44
78	Magnetic interactions in NiO at ultrahigh pressure. Physical Review B, 2016, 93, .	3.2	15
79	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:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>6</mml:mn><mml:mi>s</mml:mi></mml:mrow></mml:math>states in Cs. Physical Review B, 2016, 93, .	3.2	18
80	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
81	Lattice Vibrations Change the Solid Solubility of an Alloy at High Temperatures. Physical Review Letters, 2016, 117, 205502.	7.8	60
82	Changes in work function due to <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>NO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>adsorption on monolayer and bilayer epitaxial graphene on SiC(0001). Physical Review B, 2016, 94, .	3.2	16
83	Magnetic collapse and the behavior of transition metal oxides at high pressure. Physical Review B, 2016, 94, .	3.2	47
84	Electronic correlations in Fe at Earth's inner core conditions: Effects of alloying with Ni. Physical Review B, 2015, 91, .	3.2	12
85	Large piezoelectric response of quarternary wurtzite nitride alloys and its physical origin from first principles. Physical Review B, 2015, 92, .	3.2	41
86	Optical properties and Zeeman spectroscopy of niobium in silicon carbide. Physical Review B, 2015, 92, .	3.2	6
87	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></mml:mrow></mml:math>-SiC via nitrogen intercalation. Physical Review B, 2015, 92, .	3.2	29
88	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
89	Temperature-dependent elastic properties of Ti1âˆ’xAlxN alloys. Applied Physics Letters, 2015, 107, .	3.3	46
90	Role of N defects in paramagnetic CrN at finite temperatures from first principles. Physical Review B, 2015, 91, .	3.2	30

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91	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
92	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:msub><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
93	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:math>silicon carbide: A potential quantum bit. Physical Review B, 2015, 91, .	3.2	50
94	Morphology transition mechanism from icosahedral to decahedral phase during growth of Cu nanoclusters. Physical Review B, 2015, 92, .	3.2	5
95	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:math>studied byab initioand classical molecular dynamics with optimized potentials. Physical Review B, 2015, 91, .	3.2	53
96	The most incompressible metal osmium at static pressures above 750 gigapascals. Nature, 2015, 525, 226-229.	27.8	159
97	High temperature phase decomposition in TixZryAlzN. AIP Advances, 2014, 4, .	1.3	13
98	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
99	Vibrational free energy and phase stability of paramagnetic and antiferromagnetic CrN fromab initiomolecular dynamics. Physical Review B, 2014, 89, .	3.2	46
100	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
101	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
102	Including the effects of pressure and stress in thermodynamic functions. Physica Status Solidi (B): Basic Research, 2014, 251, 81-96.	1.5	25
103	Ab initiocalculation of the solution enthalpies of substitutional and interstitial impurities in paramagnetic fcc Fe. Physical Review B, 2014, 90, .	3.2	38
104	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></mml:math>for the treatment of localized orbitals. Physical Review B, 2014, 90, .	3.2	46
105	Electrically and Mechanically Tunable Electron Spins in Silicon Carbide Color Centers. Physical Review Letters, 2014, 112, 187601.	7.8	152
106	Temperature-dependent effective third-order interatomic force constants from first principles. Physical Review B, 2013, 88, .	3.2	266
107	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
108	Importance of Correlation Effects in hcp Iron Revealed by a Pressure-Induced Electronic Topological Transition. Physical Review Letters, 2013, 110, 117206.	7.8	58

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109	Role of screening in the density functional applied to transition-metal defects in semiconductors. Physical Review B, 2013, 87, .	3.2	35
110	Temperature dependent effective potential method for accurate free energy calculations of solids. Physical Review B, 2013, 87, .	3.2	397
111	Electronic properties and magnetism of iron at the Earth's inner core conditions. Physical Review B, 2013, 87, .	3.2	42
112	Magnetic Self-Organized Atomic Laminate from First Principles and Thin Film Synthesis. Physical Review Letters, 2013, 110, 195502.	7.8	146
113	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 50 587 Td (xmlns:mml="ht calculations. Physical Review B, 2013, 87, .	3.2	19
114	Temperature dependence of TiN elastic constants fromab initiomolecular dynamics simulations. Physical Review B, 2013, 87, .	3.2	78
115	Strong electron correlations stabilize paramagnetic cubic Cr1âˆ’xAlxN solid solutions. Applied Physics Letters, 2013, 102, .	3.3	28
116	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
117	High pressure and high temperature stabilization of cubic AlN in Ti0.60Al0.40N. Journal of Applied Physics, 2013, 113, .	2.5	34
118	The Application of Method of Exact MT-orbitals for Modelling of Thermodynamic and Mechanical Properties in Pure Components of Ti- and Zr-Based Alloys. Progress in Physics of Metals, 2013, 14, 319-352.	1.5	0
119	ab initioelastic tensor of cubic Ti<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,	3.2	125
120	Equation of state of paramagnetic CrN fromab initiomolecular dynamics. Physical Review B, 2012, 85, .	3.2	70
121	Influence of Ni on the lattice stability of Fe-Ni alloys at multimegabar pressures. Physical Review B, 2012, 86, .	3.2	1
122	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
123	Lattice dynamics of anharmonic solids from first principles. Physical Review B, 2011, 84, .	3.2	482
124	Phase Stability and Elasticity of TiAlN. Materials, 2011, 4, 1599-1618.	2.9	80
125	Impact of lattice vibrations on equation of state of the hardest boron phase. Physical Review B, 2011, 83, .	3.2	13
126	Interface core-level shifts as a probe of embedded thin-film quality. Physical Review B, 2011, 84, .	3.2	3

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127	Improving thermal stability of hard coating films via a concept of multicomponent alloying. Applied Physics Letters, 2011, 99, .	3.3	95
128	Missing-atom structure of diamondÎ£5 (001) twist grain boundary. Physical Review B, 2011, 84, .	3.2	2
129	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
130	First-principles study of dislocations in hcp metals through the investigation of the (<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 6 twin boundary. Physical Review B, 2011, 84, .	3.2	49
131	Effect of pressure on phase stability in Fe-Cr alloys. Physical Review B, 2011, 84, .	3.2	20
132	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
133	<mml:math 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></mml:msub><mml:mrow Ab initio calculations and synthesis of the off-stoichiometric half-Heusler phase Ni1â^’xMn1+xSb. Journal of Applied Physics, 2010, 108, 093712.	2.5	10
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