Mojmir Sob

List of Publications by Year
in descending order

214 papers	4,761 citations	87888 38 h-index	144013 57 g-index
215 all docs	215 docs citations	215 times ranked	2992 citing authors

#	Article	IF	Citations
1	Electronic Structure of Disordered Alloys, Surfaces and Interfaces. , 1997, , .		401
2	Interfacial segregation and grain boundary embrittlement: An overview and critical assessment of experimental data and calculated results. Progress in Materials Science, 2017, 87, 83-139.	32.8	160
3	Magnetic properties of the CrMnFeCoNi high-entropy alloy. Physical Review B, 2017, 96, .	3.2	124
4	The effect of segregated sp-impurities on grain-boundary and surface structure, magnetism and embrittlement in nickel. Progress in Materials Science, 2011, 56, 817-840.	32.8	118
5	Theoretical tensile stress in tungsten single crystals by full-potential first-principles calculations. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 1997, 234-236, 1075-1078.	5.6	116
6	Ab initio calculations of mechanical properties: Methods and applications. Progress in Materials Science, 2015, 73, 127-158.	32.8	114
7	Calculations of theoretical strength: State of the art and history. Journal of Computer-Aided Materials Design, 2004, 11, 1-28.	0.7	101
8	Thermal vacancies and positron-lifetime measurements inFe76.3Al23.7. Physical Review B, 1990, 41, 11869-11874.	3.2	92
9	Ab initiocalculation of phase boundaries in iron along the bcc-fcc transformation path and magnetism of iron overlayers. Physical Review B, 2001, 63, .	3.2	91
10	Evaluation of some basic positron-related characteristics of SiC. Physical Review B, 1996, 54, 2512-2517.	3.2	89
11	Interatomic forces and atomic structure of grain boundaries in copper-bismuth alloys. Physical Review B, 1993, 47, 5571-5582.	3.2	86
12	Interlayer magnetic coupling: Effect of interface roughness. Physical Review B, 1996, 53, 5125-5128.	3.2	78
13	Local stability of higher-energy phases in metallic materials and its relation to the structure of extended defects. Computational Materials Science, 1997, 8, 100-106.	3.0	77
14	Ab initiocalculation of tensile strength in iron. Philosophical Magazine, 2003, 83, 3529-3537.	1.6	77
15	Ab initiocalculations of elastic and magnetic properties of Fe, Co, Ni, and Cr crystals under isotropic deformation. Physical Review B, 2003, 67, .	3.2	74
16	First-principles study of magnetism at grain boundaries in iron and nickel. Physical Review B, 2008, 78, .	3.2	73
17	Atomic structure of a grain boundary in a metallic alloy: Combined electron microscope and theoretical study. Physical Review Letters, 1991, 67, 1894-1897.	7.8	71
18	On the calculation of the surface Green function by the tight-binding linear muffin-tin orbital method. Journal of Physics Condensed Matter, 1989, 1, 9893-9897.	1.8	69

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19	The role of ab initio electronic structure calculations in studies of the strength of materials. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2004, 387-389, 148-157.	5.6	67
20	Ab initiostudy of the ideal tensile strength and mechanical stability of transition-metal disilicides. Physical Review B, 2003, 68, .	3.2	61
21	Ab initiocalculations of ideal tensile strength and mechanical stability in copper. Journal of Physics Condensed Matter, 2004, 16, 1045-1052.	1.8	61
22	First-principles calculation of positron lifetimes and affinities in perfect and imperfect transition-metal carbides and nitrides. Physical Review B, 1994, 49, 10947-10957.	3.2	57
23	Vacancies and vacancy-oxygen complexes in silicon: Positron annihilation with core electrons. Physical Review B, 1998, 58, 10475-10483.	3.2	55
24	A study of the applicability of many-body central force potentials in NiAl and TiAl. Modelling and Simulation in Materials Science and Engineering, 1999, 7, 369-381.	2.0	54
25	Why calculated energies of grain boundary segregation are unreliable when segregant solubility is low. Scripta Materialia, 2013, 68, 547-550.	5.2	53
26	Why Is Polonium Simple Cubic and So Highly Anisotropic?. Physical Review Letters, 2007, 99, 016402.	7.8	51
27	Ab initio study of formation energy and magnetism of sigma phase in Crâ€“Fe and Crâ€“Co systems. Intermetallics, 2010, 18, 212-220.	3.9	51
28	Ab initiostudy of the bcc-hcp transformation in iron. Physical Review B, 2008, 77, .	3.2	50
29	Calculation of theoretical strength of solids by linear muffin-tin orbitals (LMTO) method. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 1997, 234-236, 370-372.	5.6	49
30	Theoretical calculations of positron annihilation with rare-gas core electrons in simple and transition metals. Physical Review B, 1991, 43, 2580-2593.	3.2	48
31	Positron affinity in semiconductors: Theoretical and experimental studies. Physical Review B, 1999, 59, 1948-1955.	3.2	48
32	Ferromagnetism of Imperfect Ultrathin Ru and Rh Films on a Ag(001) Substrate. Physical Review Letters, 1995, 74, 2551-2554.	7.8	47
33	The role of higher-symmetry phases in anisotropy of theoretical tensile strength of metals and intermetallics. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1998, 78, 653-658.	0.6	47
34	Phase diagram calculations in the Coâ€“Mo and Feâ€“Mo systems using first-principles results for the sigma phase. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2005, 29, 133-139.	1.6	47
35	Structural stability of higher-energy phases and its relation to the atomic configurations of extended defects: The example of Cu. Physical Review B, 1999, 60, 844-850.	3.2	44
36	Positron annihilation in iron and B2-ordered alloys FeAl and FeTi. Journal of Physics F: Metal Physics, 1982, 12, 571-596.	1.6	43

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37	Recent trends and open questions in grain boundary segregation. Journal of Materials Research, 2018, 33, 2647-2660.	2.6	42
38	Ab initioanalysis of energetics of Ïƒ-phase formation in Cr-based systems. Physical Review B, 2001, 63, .	3.2	41
39	Instability of higher-energy phases in simple and transition metals. Journal of Physics and Chemistry of Solids, 2003, 64, 863-872.	4.0	41
40	Re-modeling of Laves phases in the Crâ€“Nb and Crâ€“Ta systems using first-principles results. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2009, 33, 179-186.	1.6	38
41	Applied Thermodynamics: Grain Boundary Segregation. Entropy, 2014, 16, 1462-1483.	2.2	38
42	Thermodynamic modeling of Laves phases in the Crâ€“Hf and Crâ€“Ti systems: Reassessment using first-principles results. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2010, 34, 215-221.	1.6	37
43	Total energy and electronic structure calculations of C15 Laves-phase compounds MV₂ (M=Zr, Hf or Ta): Elastic properties. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1994, 70, 881-892.	0.6	33
44	Magnetically dead layers at<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>s</mml:mi><mml:mi>p</mml:mi></mml:mrow></mml:math>-impurity-decorated grain boundaries and surfaces in nickel. Physical Review B, 2011, 84, .	3.2	33
45	Noncollinear magnetism in manganese nanostructures. Physical Review B, 2009, 80, .	3.2	32
46	Stability of Laves phases in the Crâ€“Zr system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2009, 33, 382-387.	1.6	30
47	Phase stability, elasticity, and theoretical strength of polonium from first principles. Physical Review B, 2010, 81, .	3.2	30
48	Positron affinity for precipitates in reactor pressure vessel steels. Nuclear Engineering and Design, 1995, 158, 149-156.	1.7	29
49	Ab initio tensile tests of grain boundaries in the fcc crystals of Ni and Co with segregated sp-impurities. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2016, 669, 218-225.	5.6	29
50	Stability and elasticity of metastable solid solutions and superlattices in the MoNâ€“TaN system: First-principles calculations. Materials and Design, 2018, 144, 310-322.	7.0	29
51	Correlating structural and mechanical properties of AlN/TiN superlattice films. Scripta Materialia, 2019, 165, 159-163.	5.2	29
52	Theory of strengthening of alpha titanium by interstitial solutes. European Physical Journal D, 1975, 25, 872-890.	0.4	28
53	An analysis of segregation-induced changes in grain boundary cohesion in bcc iron. Journal of Materials Science, 2014, 49, 2477-2482.	3.7	28
54	Phase stability of C15 MV₂ (M=Zr, Hf or Ta): An electronic structure investigation. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1998, 77, 121-136.	0.6	27

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55	Ab initio calculations of lattice stability of sigma-phase and phase diagram in the Crâ€“Fe system. Computational Materials Science, 2002, 25, 562-569.	3.0	27
56	Phase diagram calculation in Coî—¸Cr system using Ab initio determined lattice instability of sigma phase. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2002, 26, 513-522.	1.6	27
57	Determining the Elasticity of Materials Employing Quantumâ€mechanical Approaches: From the Electronic Ground State to the Limits of Materials Stability. Steel Research International, 2011, 82, 86-100.	1.8	27
58	Ab initiostudy of Co and Ni under uniaxial and biaxial loading and in epitaxial overlayers. Physical Review B, 2008, 78, .	3.2	26
59	Defect and atomic ordering studies in highly deformed and disordered Fe72Al28 alloy. Acta Materialia, 1997, 45, 2147-2154.	7.9	25
60	Ab initiodensity functional calculations of ferromagnetism in low-dimensional nanostructures: From nanowires to nanorods. Physical Review B, 2009, 79, .	3.2	24
61	Atomistic approaches to cleavage of interfaces. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 035007.	2.0	24
62	Electronic structure of random semiconductor alloys by the tight-binding linear muffin-tin orbital method. Physical Review B, 1989, 40, 10029-10032.	3.2	23
63	First-principles calculations of energetics of sigma phase formation and thermodynamic modelling in Feâ€“Niâ€“Cr system. Journal of Alloys and Compounds, 2004, 378, 71-74.	5.5	22
64	Facet-controlled phase separation in supersaturated Au-Ni nanoparticles upon shape equilibration. Applied Physics Letters, 2015, 107, .	3.3	22
65	Strength and Brittleness of Interfaces in Fe-Al Superalloy Nanocomposites under Multiaxial Loading: An ab initio and Atomistic Study. Nanomaterials, 2018, 8, 873.	4.1	22
66	Bond-Order Potentials for Molybdenum and Niobium: An Assessment of Their Quality. Materials Research Society Symposia Proceedings, 1998, 538, 529.	0.1	21
67	Entropy matters in grain boundary segregation. Acta Materialia, 2021, 206, 116597.	7.9	21
68	Electronic structure and positron annihilation in alkali metals: Isolation of ionic core contribution and valence high-momentum components. Solid State Communications, 1985, 53, 249-253.	1.9	20
69	Modelling of phase diagrams of nanoalloys with complex metallic phases: application to Niâ€“Sn. Physical Chemistry Chemical Physics, 2015, 17, 28200-28210.	2.8	20
70	Ab initiostudy of thermodynamic, electronic, magnetic, structural, and elastic properties of Ni<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>N allotropes. Physical Review B, 2013, 88, .	3.2	19
71	Origin of the Low Magnetic Moment in Fe2AlTi: An Ab Initio Study. Materials, 2018, 11, 1732.	2.9	19
72	Amplitude and Phase of the Oscillatory Exchange Coupling between Fe-Co-Ni Alloy Layers across a Cu Spacer Layer. Physical Review Letters, 1997, 78, 358-361.	7.8	18

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73	Many-body potentials for Cu-Ti intermetallic alloys and a molecular dynamics study of vitrification and amorphization. Modelling and Simulation in Materials Science and Engineering, 1993, 1, 315-333.	2.0	17
74	Ab initio study of phase transformations in transition-metal disilicides. Intermetallics, 2011, 19, 919-926.	3.9	17
75	Shear instabilities in perfect bcc crystals during simulated tensile tests. Physical Review B, 2013, 87, .	3.2	17
76	An ab initio study of mechanical and dynamical stability of MoSi2. Journal of Alloys and Compounds, 2018, 746, 720-728.	5.5	17
77	The effect of structural degrees of freedom on bonding and strength characteristics of molybdenum disilicide. Intermetallics, 2009, 17, 523-528.	3.9	16
78	Ab initio study of C14 laves phases in Fe-based systems. Journal of Mining and Metallurgy, Section B: Metallurgy, 2012, 48, 395-401.	0.8	16
79	Systematics of the rare-gas core contributions to the positron annihilation spectra of some simple and transition metals. Solid State Communications, 1985, 53, 255-258.	1.9	15
80	Ab initiostudy of energetics and magnetism of Fe, Co, and Ni along the trigonal deformation path. Physical Review B, 2011, 83, .	3.2	15
81	Impact of Nano-Scale Distribution of Atoms on Electronic and Magnetic Properties of Phases in Fe-Al Nanocomposites: An Ab Initio Study. Nanomaterials, 2018, 8, 1059.	4.1	15
82	Electron-positron interaction in metals: momentum dependence of HMC and ionic core enhancement factors. Journal of Physics Condensed Matter, 1989, 1, 6321-6326.	1.8	14
83	High sensitivity of umklapp components of momentum densities to the crystal potential and its consequences for the electron-positron enhancement factor. Physical Review B, 1990, 41, 10529-10534.	3.2	14
84	Mechanical stability of Ni and Ir under hydrostatic and uniaxial loading. Modelling and Simulation in Materials Science and Engineering, 2015, 23, 055010.	2.0	14
85	Atomistic Modelingâ€Based Design of Novel Materials. Advanced Engineering Materials, 2017, 19, 1600688.	3.5	14
86	Tensorial elastic properties and stability of interface states associated with Î£5(210) grain boundaries in Ni3(Al,Si). Science and Technology of Advanced Materials, 2017, 18, 273-282.	6.1	14
87	Quantum-Mechanical Study of Nanocomposites with Low and Ultra-Low Interface Energies. Nanomaterials, 2018, 8, 1057.	4.1	13
88	An Ab Initio Study of Pressure-Induced Changes of Magnetism in Austenitic Stoichiometric Ni2MnSn. Materials, 2021, 14, 523.	2.9	13
89	Theoretical calculations of positron annihilation characteristics in inorganic solids â€" Recent advances and problems. Advances in Quantum Chemistry, 2003, , 77-108.	0.8	12
90	Segregation ofsp-impurities at grain boundaries and surfaces: comparison of fcc cobalt and nickel. Modelling and Simulation in Materials Science and Engineering, 2017, 25, 085004.	2.0	12

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91	An Ab Initio Study of Thermodynamic and Mechanical Stability of Heusler-Based Fe2AlCo Polymorphs. Materials, 2018, 11, 1543.	2.9	12
92	Effect of high pressure on magnetic properties of CrMnFeCoNi high entropy alloy. Journal of Magnetism and Magnetic Materials, 2019, 487, 165333.	2.3	12
93	Polarized Positron Annihilation and Enhancement Effects in Ferromagnetic Iron. Physica Status Solidi (B): Basic Research, 1984, 123, 649-652.	1.5	11
94	A First-Principles Tight-Binding Method for Electronic Structure Calculations in Amorphous Solids*. Zeitschrift Fur Physikalische Chemie, 1988, 157, 515-520.	2.8	11
95	Theoretical studies of epitaxially grown Co and Ni thin films on (111) metallic substrates. Physical Review B, 2008, 77, .	3.2	11
96	Application of Ab Initio Electronic Structure Calculations in Construction of Phase Diagrams of Metallic Systems with Complex Phases. Solid State Phenomena, 2009, 150, 1-28.	0.3	11
97	Ab initio study of deformed As, Sb, and Bi with an application to thin films. Physical Review B, 2016, 94, .	3.2	11
98	Elasticity of Phases in Fe-Al-Ti Superalloys: Impact of Atomic Order and Anti-Phase Boundaries. Crystals, 2019, 9, 299.	2.2	11
99	An Ab Initio Study of Vacancies in Disordered Magnetic Systems: A Case Study of Fe-Rich Fe-Al Phases. Materials, 2019, 12, 1430.	2.9	11
100	Point-defect engineering of MoN/TaN superlattice films: A first-principles and experimental study. Materials and Design, 2020, 186, 108211.	7.0	11
101	Electronic structure and positron annihilation in B2-ordered CuZn. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1983, 48, 523-535.	0.6	10
102	Electron momentum density and the momentum density of positron annihilation pairs in alkali metals: high-momentum components. Journal of Physics F: Metal Physics, 1985, 15, 1685-1691.	1.6	10
103	Theoretical Strength of Metals and Intermetallics from First Principles. Materials Science Forum, 2005, 482, 33-38.	0.3	10
104	Application of ab initio electronic structure calculations for prediction of phase equilibria in superaustenitic steels. Computational Materials Science, 2006, 38, 298-302.	3.0	10
105	Energetics and phase diagrams of Fe-Cr and Co-Cr systems from first principles. Journal of Mining and Metallurgy, Section B: Metallurgy, 2002, 38, 205-211.	0.8	10
106	Electronic effects in the order-disorder transition in Î² brass. Journal of Physics F: Metal Physics, 1988, 18, 2387-2408.	1.6	9
107	On various possibilities of interpretation of the effective enhancement factor in positron annihilation. Journal of Physics F: Metal Physics, 1988, 18, 1317-1328.	1.6	9
108	Positron annihilation in vacancies at grain boundaries in metals. Applied Surface Science, 2008, 255, 128-131.	6.1	9

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109	Combined quantum-mechanical and Calphad approach to description of heat capacity of pure elements below room temperature. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2015, 51, 161-171.	1.6	9
110	The theoretical and experimental study of the Sb-Sn nano-alloys. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2019, 64, 90-96.	1.6	9
111	Multi-phase ELAStic Aggregates (MELASA) software tool for modeling anisotropic elastic properties of lamellar composites. Computer Physics Communications, 2020, 247, 106863.	7.5	9
112	Sessile Splittings of Screw Dislocations in H.C.P. Metals. Physica Status Solidi A, 1974, 24, K133-K136.	1.7	8
113	Higher-energy Structures and Stability of Cu and Al Crystals Along Displacive Transformation Paths. Journal of Computer-Aided Materials Design, 2006, 12, 161-173.	0.7	8
114	A peculiar bonding of sulphur at the Nb(001) surface. Europhysics Letters, 2008, 83, 26001.	2.0	8
115	Laves phases in the Vâ€“Zr system below room temperature: Stability analysis using ab initio results and phase diagram. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2014, 44, 62-69.	1.6	8
116	Theoretical investigations on structural, elastic, thermodynamic and electronic properties of Al₃Ti and Al₃V compounds in L1₂ structure under high pressure. Materials Research Express, 2019, 6, 056536.	1.6	8
117	Phase Stability of Iron Nitride Fe4N at High Pressureâ€”Pressure-Dependent Evolution of Phase Equilibria in the Feâ€“N System. Materials, 2021, 14, 3963.	2.9	8
118	The Cost of Improving the Precision of the Variational Quantum Eigensolver for Quantum Chemistry. Nanomaterials, 2022, 12, 243.	4.1	8
119	Phase stability and elasticity of C15 transition-metal intermetallic compounds. Journal of Phase Equilibria and Diffusion, 1997, 18, 536-543.	0.3	7
120	First-principles calculations of energetics of sigma phase formation and thermodynamic modelling in the Crâ€“Feâ€“W system. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2007, 462, 153-158.	5.6	7
121	Characterization of iron ferromagnetism by the local atomic volume: from three-dimensional structures to isolated atoms. Journal of Physics Condensed Matter, 2014, 26, 086002.	1.8	7
122	Ab initiostudy of energetics and magnetism of sigma phase in Coâ€“Mo and Feâ€“Mo systems. Modelling and Simulation in Materials Science and Engineering, 2016, 24, 025009.	2.0	7
123	A Quantumâ€“Mechanical Study of Clean and Crâ€“Segregated Antiphase Boundaries in Fe3Al. Materials, 2019, 12, 3954.	2.9	7
124	Positron Annihilation Characteristics in Perfect and Imperfect Transition Metal Carbides and Nitrides. European Physical Journal Special Topics, 1995, 05, C1-135-C1-142.	0.2	7
125	The Determination of Ionic Radii of Some Metals by the Positron Annihilation Method. Physica Status Solidi (B): Basic Research, 1976, 73, K1.	1.5	6
126	Spin-polarized positron annihilation and magnetic moment in Fe1â^'xCox alloys. Journal of Magnetism and Magnetic Materials, 1986, 62, 202-204.	2.3	6

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127	First-principles calculations of electronic structure in random hcp alloys: A Ru-Re example. Physical Review B, 1990, 41, 10459-10462.	3.2	6
128	Positron annihilation at grain boundaries in metals. Physica Status Solidi C: Current Topics in Solid State Physics, 2007, 4, 3461-3464.	0.8	6
129	Åob, Legut, and FriÃ¡k Reply:. Physical Review Letters, 2009, 102, .	7.8	6
130	Theoretical analysis of dislocation splittings in MoSi₂. Journal of Physics: Conference Series, 2010, 240, 012007.	0.4	6
131	Quantum-mechanical study of tensorial elastic and high-temperature thermodynamic properties of grain boundary states in superalloy-phase Ni3Al. IOP Conference Series: Materials Science and Engineering, 2017, 219, 012019.	0.6	6
132	Impact of Antiphase Boundaries on Structural, Magnetic and Vibrational Properties of Fe3Al. Materials, 2020, 13, 4884.	2.9	6
133	An Ab Initio Study of Magnetism in Disordered Fe-Al Alloys with Thermal Antiphase Boundaries. Nanomaterials, 2020, 10, 44.	4.1	6
134	The Effect of Vacancies on Grain Boundary Segregation in Ferromagnetic fcc Ni. Nanomaterials, 2020, 10, 691.	4.1	6
135	Modelling of phase equilibria in the Hf-V system below room temperature. Journal of Mining and Metallurgy, Section B: Metallurgy, 2017, 53, 239-247.	0.8	6
136	Pressure-Induced Increase of the Total Magnetic Moment in Ferrimagnetic Ni_{1.9375}Mn_{1.5625}Sn_{0.5} Martensite: A Quantum-Mechanical Study. Materials Transactions, 2022, 63, 430-435.	1.2	6
137	Study of Point Defects in Silicon by Means of Positron Annihilation with Core Electrons. Materials Science Forum, 1997, 255-257, 605-607.	0.3	5
138	Study of the Mechanical Behavior of BCC Transition Metals Using Bond-Order Potentials. Materials Research Society Symposia Proceedings, 1999, 578, 199.	0.1	5
139	Sensitivity of electron and electron-positron momentum densities to various electron and positron crystal potentials. Physical Review B, 2001, 64, .	3.2	5
140	The Role of Ab Initio Electronic Structure Calculations in Contemporary Materials Science. Key Engineering Materials, 2002, 227, 261-0.	0.4	5
141	Magnetism of Ni3Al and Fe3Al under extreme pressure and shape deformation: an ab initio study. Journal of Magnetism and Magnetic Materials, 2004, 272-276, E205-E206.	2.3	5
142	Planar defects and dislocations in transition-metal disilicides. Intermetallics, 2015, 58, 43-49.	3.9	5
143	Magnetism and deformation of epitaxial Pd and Rh thin films. Physical Review B, 2016, 93, .	3.2	5
144	Ab initio study of chemical disorder as an effective stabilizing mechanism of bcc-based <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>TiAl</mml:mi><mml:mo>(</mml:mo><mml:mo>+</mml:mo><mml:mi> 2020, 4, .	2.4	5

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145	High strain rate deformation and positron annihilation in Fe-3.5wt.%Si single crystals. Materials Science and Engineering, 1984, 65, L9-L12.	0.1	4
146	An efficient method for calculation of electronic charge and spin densities in perfect and perturbed crystalline solids. Journal of Physics F: Metal Physics, 1986, 16, 577-584.	1.6	4
147	Electronic structure in random hexagonal close-packed transition-metal alloys by the tight-binding linear-muffin-tin-orbital coherent-potential method. Physical Review B, 1991, 43, 4622-4628.	3.2	4
148	Ideal Tensile Strength of Ni₃Al and Fe₃Al with D0₃ Structure. Materials Science Forum, 2008, 567-568, 77-80.	0.3	4
149	Stacking Faults and Dislocation Dissociation in MoSi2. Materials Research Society Symposia Proceedings, 2008, 1128, 71001.	0.1	4
150	Mechanical and magnetic properties of Mn-Pt compounds and nanocomposites. Physical Review B, 2012, 85, .	3.2	4
151	An Ab Initio Study of Connections between Tensorial Elastic Properties and Chemical Bonds in Î£5(210) Grain Boundaries in Ni3Si. Materials, 2018, 11, 2263.	2.9	4
152	Self-Consistent Greenâ€²s Function Method for Random Surfaces and Interfaces. NATO ASI Series Series B: Physics, 1996, , 237-264.	0.2	4
153	Positron annihilation in some transition metal oxides. Physics Letters, Section A: General, Atomic and Solid State Physics, 1975, 53, 65-66.	2.1	3
154	Investigation of the surface of vanadium single crystals by positron annihilation. Physica Status Solidi (B): Basic Research, 1978, 90, K1.	1.5	3
155	Scalar fields around a charged, rotating black hole. European Physical Journal D, 1978, 28, 121-124.	0.4	3
156	Determination of electronic momentum densities and the Fermi surface of white tin by positron annihilation. European Physical Journal D, 1979, 29, 1124-1135.	0.4	3
157	Positron Annihilation and MÃ¶ssbauer Spectroscopy in Highly Strained Fe₇₂Al₂₈ Alloy. Materials Science Forum, 1995, 175-178, 399-402.	0.3	3
158	Interlayer magnetic coupling: Effect of disorder in spacer. Journal of Magnetism and Magnetic Materials, 1996, 156, 245-246.	2.3	3
159	Spinâ€“orbit coupling in lowâ€dimensional gold. Physica Status Solidi - Rapid Research Letters, 2008, 2, 117-119.	2.4	3
160	A mechanism of inhibition of phase transitions in nano-grained close-packed Pd thin films. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2010, 34, 421-427.	1.6	3
161	Ab initio study of the theoretical strength and magnetism of the Feâˆ’Pd, Feâˆ’Pt and Feâˆ’Cu nanocomposites. Journal of Magnetism and Magnetic Materials, 2019, 469, 100-107.	2.3	3
162	Surface-induced magnetism in intermetallics: Ni3Ge compound as a case study. Journal of Magnetism and Magnetic Materials, 2019, 474, 273-281.	2.3	3

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163	Quantum-Mechanical Assessment of the Energetics of Silver Decahedron Nanoparticles. Nanomaterials, 2020, 10, 767.	4.1	3
164	The Effect of Hydrogen on the Stress-Strain Response in Fe3Al: An ab initio Molecular-Dynamics Study. Materials, 2021, 14, 4155.	2.9	3
165	The Impact of Vibrational Entropy on the Segregation of Cu to Antiphase Boundaries in Fe3Al. Magnetochemistry, 2021, 7, 108.	2.4	3
166	On the Role of Nonâ€"Pair Potential Terms in Semiempirical Quantumâ€"Mechanical Simulations. NATO ASI Series Series B: Physics, 1996, , 449-454.	0.2	3
167	Impact of Disorder on Properties of Vacancies: A Case Study of B2 and A2 Polymorphs of Non-Stoichiometric Fe2CoAl. Crystals, 2021, 11, 1207.	2.2	3
168	Investigation of Defects and Atomic Ordering in Fe72Al28 by Positron Annihilation and MÃ¶ssbauer Spectroscopy. European Physical Journal Special Topics, 1995, 05, C1-157-C1-161.	0.2	3
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