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	The Cost of Improving the Precision of the Variational Quantum Eigensolver for Quantum Chemistry. Nanomaterials, 2022, 12, 243.	4.1	8
2	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
3	Best-Practice Aspects of Quantum-Computer Calculations: A Case Study of the Hydrogen Molecule. Molecules, 2022, 27, 597.	3.8	3
4	An Ab Initio Study of Pressure-Induced Changes of Magnetism in Austenitic Stoichiometric Ni2MnSn. Materials, 2021, 14, 523.	2.9	13
5	Entropy matters in grain boundary segregation. Acta Materialia, 2021, 206, 116597.	7.9	21
6	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
7	The Effect of Hydrogen on the Stress-Strain Response in Fe3Al: An ab initio Molecular-Dynamics Study. Materials, 2021, 14, 4155.	2.9	3
8	The Impact of Vibrational Entropy on the Segregation of Cu to Antiphase Boundaries in Fe3Al. Magnetochemistry, 2021, 7, 108.	2.4	3
9	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
10	A Quantum-Mechanical Study of Antiphase Boundaries in Ferromagnetic B2-Phase Fe2CoAl Alloy. Magnetochemistry, 2021, 7, 137.	2.4	2
11	AB INITIO STUDY OF SILVER NANOPARTICLES, GRAIN BOUNDARIES AND THEIR QUADRUPLE JUNCTIONS. , 2021, , .		0
12	ANOMALOUS PRESSURE-INDUCED CHANGES IN MAGNETISM OF FERRIMAGNETIC Ni-Mn-Sn STRUCTURES. , 2021, , .		0
13	Multi-phase ELAStic Aggregates (MELASA) software tool for modeling anisotropic elastic properties of lamellar composites. Computer Physics Communications, 2020, 247, 106863.	7.5	9
14	Point-defect engineering of MoN/TaN superlattice films: A first-principles and experimental study. Materials and Design, 2020, 186, 108211.	7.0	11
15	Impact of Antiphase Boundaries on Structural, Magnetic and Vibrational Properties of Fe3Al. Materials, 2020, 13, 4884.	2.9	6
16	Editorial for the Special Issue on Computational Quantum Physics and Chemistry of Nanomaterials. Nanomaterials, 2020, 10, 2395.	4.1	0
17	An Ab Initio Study of Magnetism in Disordered Fe-Al Alloys with Thermal Antiphase Boundaries. Nanomaterials, 2020, 10, 44.	4.1	6
18	Quantum-Mechanical Assessment of the Energetics of Silver Decahedron Nanoparticles. Nanomaterials, 2020, 10, 767.	4.1	3

#	Article	IF	Citations
19	The Effect of Vacancies on Grain Boundary Segregation in Ferromagnetic fcc Ni. Nanomaterials, 2020, 10, 691.	4.1	6
20	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>+2.4</mml:mo><mml:mi> 2020, 4, .	2.4	5
21	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
22	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
23	Elasticity of Phases in Fe-Al-Ti Superalloys: Impact of Atomic Order and Anti-Phase Boundaries. Crystals, 2019, 9, 299.	2.2	11
24	Effect of high pressure on magnetic properties of CrMnFeCoNi high entropy alloy. Journal of Magnetism and Magnetic Materials, 2019, 487, 165333.	2.3	12
25	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
26	Correlating structural and mechanical properties of AlN/TiN superlattice films. Scripta Materialia, 2019, 165, 159-163.	5.2	29
27	Atomistic approaches to cleavage of interfaces. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 035007.	2.0	24
28	A Quantumâ€“Mechanical Study of Clean and Crâ€“Segregated Antiphase Boundaries in Fe3Al. Materials, 2019, 12, 3954.	2.9	7
29	Professor Jan VÅ™eÅ¡Å¥Ã¡l and His Contributions Towards the Implementing of Ab Initio Data into the CALPHAD Method and Extension of the Phase Diagram Calculations Down to 0ÂK. Journal of Phase Equilibria and Diffusion, 2019, 40, 3-9.	1.4	0
30	Surface-induced magnetism in intermetallics: Ni3Ge compound as a case study. Journal of Magnetism and Magnetic Materials, 2019, 474, 273-281.	2.3	3
31	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
32	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
33	An ab initio study of mechanical and dynamical stability of MoSi2. Journal of Alloys and Compounds, 2018, 746, 720-728.	5.5	17
34	Dislocation dissociations in C11b MoSi2 and their impact on its plastic deformation. Intermetallics, 2018, 97, 34-41.	3.9	2
35	Study of Local Mechanical Properties of Fe₇₈Al₂₂ Alloy. Key Engineering Materials, 2018, 784, 27-32.	0.4	1
36	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

#	Article	IF	Citations
37	Origin of the Low Magnetic Moment in Fe2AlTi: An Ab Initio Study. Materials, 2018, 11, 1732.	2.9	19
38	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
39	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
40	An Ab Initio Study of Pressure-Induced Reversal of Elastically Stiff and Soft Directions in YN and ScN and Its Effect in Nanocomposites Containing These Nitrides. Nanomaterials, 2018, 8, 1049.	4.1	2
41	Quantum-Mechanical Study of Nanocomposites with Low and Ultra-Low Interface Energies. Nanomaterials, 2018, 8, 1057.	4.1	13
42	An Ab Initio Study of Thermodynamic and Mechanical Stability of Heusler-Based Fe2AlCo Polymorphs. Materials, 2018, 11, 1543.	2.9	12
43	Recent trends and open questions in grain boundary segregation. Journal of Materials Research, 2018, 33, 2647-2660.	2.6	42
44	Atomistic Modelingâ€Based Design of Novel Materials. Advanced Engineering Materials, 2017, 19, 1600688.	3.5	14
45	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
46	Magnetic properties of the CrMnFeCoNi high-entropy alloy. Physical Review B, 2017, 96, .	3.2	124
47	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
48	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
49	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
50	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
51	Ab initio study of deformed As, Sb, and Bi with an application to thin films. Physical Review B, 2016, 94, .	3.2	11
52	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
53	Magnetism and deformation of epitaxial Pd and Rh thin films. Physical Review B, 2016, 93, .	3.2	5
54	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

#	Article	IF	Citations
55	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
56	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
57	Facet-controlled phase separation in supersaturated Au-Ni nanoparticles upon shape equilibration. Applied Physics Letters, 2015, 107, .	3.3	22
58	Ab initio calculations of mechanical properties: Methods and applications. Progress in Materials Science, 2015, 73, 127-158.	32.8	114
59	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
60	Planar defects and dislocations in transition-metal disilicides. Intermetallics, 2015, 58, 43-49.	3.9	5
61	What Types of Stacking Faults and Dislocation Dissociations Can Be Found in Transition-Metal Disilicides. Acta Physica Polonica A, 2015, 128, 589-592.	0.5	0
62	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
63	Applied Thermodynamics: Grain Boundary Segregation. Entropy, 2014, 16, 1462-1483.	2.2	38
64	An analysis of segregation-induced changes in grain boundary cohesion in bcc iron. Journal of Materials Science, 2014, 49, 2477-2482.	3.7	28
65	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
66	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
67	Why calculated energies of grain boundary segregation are unreliable when segregant solubility is low. Scripta Materialia, 2013, 68, 547-550.	5.2	53
68	Shear instabilities in perfect bcc crystals during simulated tensile tests. Physical Review B, 2013, 87, .	3.2	17
69	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
70	Mechanical and magnetic properties of Mn-Pt compounds and nanocomposites. Physical Review B, 2012, 85, .	3.2	4
71	Application of Ab Initio Results in Modeling Phase Diagrams Containing Complex Phases. Journal of Solid Mechanics and Materials Engineering, 2012, 6, 39-47.	0.5	1
72	Ab initio study of phase transformations in transition-metal disilicides. Intermetallics, 2011, 19, 919-926.	3.9	17

#	Article	IF	Citations
73	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
74	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
75	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
76	Ab initiostudy of energetics and magnetism of Fe, Co, and Ni along the trigonal deformation path. Physical Review B, 2011, 83, .	3.2	15
77	Phase stability, elasticity, and theoretical strength of polonium from first principles. Physical Review B, 2010, 81, .	3.2	30
78	Theoretical analysis of dislocation splittings in MoSi₂. Journal of Physics: Conference Series, 2010, 240, 012007.	0.4	6
79	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
80	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
81	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
82	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
83	Åob, Legut, and FriÃ¡k Reply:. Physical Review Letters, 2009, 102, .	7.8	6
84	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
85	Stability of Laves phases in the Crâ€“Zr system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2009, 33, 382-387.	1.6	30
86	The effect of structural degrees of freedom on bonding and strength characteristics of molybdenum disilicide. Intermetallics, 2009, 17, 523-528.	3.9	16
87	Noncollinear magnetism in manganese nanostructures. Physical Review B, 2009, 80, .	3.2	32
88	Ab initiodensity functional calculations of ferromagnetism in low-dimensional nanostructures: From nanowires to nanorods. Physical Review B, 2009, 79, .	3.2	24
89	Ideal Tensile Strength of Ni₃Al and Fe₃Al with D0₃ Structure. Materials Science Forum, 2008, 567-568, 77-80.	0.3	4
90	Positron annihilation in vacancies at grain boundaries in metals. Applied Surface Science, 2008, 255, 128-131.	6.1	9

#	Article	IF	Citations
91	Spinâ€“orbit coupling in lowâ€dimensional gold. Physica Status Solidi - Rapid Research Letters, 2008, 2, 117-119.	2.4	3
92	A peculiar bonding of sulphur at the Nb(001) surface. Europhysics Letters, 2008, 83, 26001.	2.0	8
93	Theoretical studies of epitaxially grown Co and Ni thin films on (111) metallic substrates. Physical Review B, 2008, 77, .	3.2	11
94	Ab initiostudy of the bcc-hcp transformation in iron. Physical Review B, 2008, 77, .	3.2	50
95	Ab initiostudy of Co and Ni under uniaxial and biaxial loading and in epitaxial overlayers. Physical Review B, 2008, 78, .	3.2	26
96	First-principles study of magnetism at grain boundaries in iron and nickel. Physical Review B, 2008, 78, .	3.2	73
97	Most pressurized elements arenâ€™t simple cubic. Physics Today, 2008, 61, 10-11.	0.3	2
98	Stacking Faults and Dislocation Dissociation in MoSi2. Materials Research Society Symposia Proceedings, 2008, 1128, 71001.	0.1	4
99	The role of ab initio electronic structure calculations in multiscale modelling of materials. , 2007, , 1-24.		0
100	Why Is Polonium Simple Cubic and So Highly Anisotropic?. Physical Review Letters, 2007, 99, 016402.	7.8	51
101	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
102	Positron annihilation at grain boundaries in metals. Physica Status Solidi C: Current Topics in Solid State Physics, 2007, 4, 3461-3464.	0.8	6
103	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
104	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
105	Theoretical Strength, Magnetism and Stability of Metals and Intermetallics. , 2005, , 307-325.		0
106	Theoretical Strength of Metals and Intermetallics from First Principles. Materials Science Forum, 2005, 482, 33-38.	0.3	10
107	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
108	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

#	Article	IF	Citations
109	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
110	Calculations of theoretical strength: State of the art and history. Journal of Computer-Aided Materials Design, 2004, 11, 1-28.	0.7	101
111	First-Principles Calculations of Energetics of Sigma Phase Formation and Thermodynamic Modelling in Feâ€"Niâ€"Cr System. ChemInform, 2004, 35, no.	0.0	0
112	Ab initiocalculations of ideal tensile strength and mechanical stability in copper. Journal of Physics Condensed Matter, 2004, 16, 1045-1052.	1.8	61
113	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
114	Instability of higher-energy phases in simple and transition metals. Journal of Physics and Chemistry of Solids, 2003, 64, 863-872.	4.0	41
115	Theoretical calculations of positron annihilation characteristics in inorganic solids â€" Recent advances and problems. Advances in Quantum Chemistry, 2003, , 77-108.	0.8	12
116	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
117	Ab initiostudy of the ideal tensile strength and mechanical stability of transition-metal disilicides. Physical Review B, 2003, 68, .	3.2	61
118	Ab initiocalculation of tensile strength in iron. Philosophical Magazine, 2003, 83, 3529-3537.	1.6	77
119	The Role of Ab Initio Electronic Structure Calculations in Contemporary Materials Science. Key Engineering Materials, 2002, 227, 261-0.	0.4	5
120	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
121	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
122	Ab Initio Study of Iron Magnetism Along Bainâ€™s Path. , 2002, , 399-415.		2
123	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
124	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
125	Excessive Sensitivity of Momentum Densities to Crystal Potentials as a Reason for Difficulties in Verifying Positron Enhancement Theories. Materials Science Forum, 2001, 363-365, 612-614.	0.3	2
126	Sensitivity of electron and electron-positron momentum densities to various electron and positron crystal potentials. Physical Review B, 2001, 64, .	3.2	5

#	Article	IF	Citations
127	Ab initioanalysis of energetics of Ïƒ-phase formation in Cr-based systems. Physical Review B, 2001, 63, .	3.2	41
128	Ab initio simulation of a tensile test in MoSi2 and WSi2. Materials Research Society Symposia Proceedings, 2000, 646, 257.	0.1	2
129	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
130	Positron affinity in semiconductors: Theoretical and experimental studies. Physical Review B, 1999, 59, 1948-1955.	3.2	48
131	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
132	Study of the Mechanical Behavior of BCC Transition Metals Using Bond-Order Potentials. Materials Research Society Symposia Proceedings, 1999, 578, 199.	0.1	5
133	Preferential Positron Annihilation in Binary Alloys. Acta Physica Polonica A, 1999, 95, 605-611.	0.5	1
134	ATOMIC-LEVEL DESCRIPTION OF MATERIAL STRENGTH OF Î±-Fe. Zairyo/Journal of the Society of Materials Science, Japan, 1999, 48, 225-233.	0.2	1
135	Application of Surface Ab Initio Methods to Studies of Electronic Structure and Atomic Configuration of Interfaces in Metallic Materials. Materials Science Forum, 1998, 294-296, 17-26.	0.3	1
136	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
137	Vacancies and vacancy-oxygen complexes in silicon: Positron annihilation with core electrons. Physical Review B, 1998, 58, 10475-10483.	3.2	55
138	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
139	AB Initio Study of Changes in the Magnetism of Iron During the BCC-HCP Phase Transformation. Materials Research Society Symposia Proceedings, 1998, 538, 523.	0.1	1
140	Bond-Order Potentials for Molybdenum and Niobium: An Assessment of Their Quality. Materials Research Society Symposia Proceedings, 1998, 538, 529.	0.1	21
141	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
142	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
143	Green Function Method. , 1997, , 59-112.		1
144	Electronic Structure, Atomic Configuration and Positron Annihilation Spectroscopy of Extended Defects in Metals. Materials Science Forum, 1997, 255-257, 420-422.	0.3	0

#	Article	IF	Citations
145	Electronic Structure and Atomic Configuration of Extended Defects in Metals by First-Principles and Semiempirical TB-LMTO Methods. Materials Research Society Symposia Proceedings, 1997, 491, 79.	0.1	0
146	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
147	Phase stability and elasticity of C15 transition-metal intermetallic compounds. Journal of Phase Equilibria and Diffusion, 1997, 18, 536-543.	0.3	7
148	Defect and atomic ordering studies in highly deformed and disordered Fe72Al28 alloy. Acta Materialia, 1997, 45, 2147-2154.	7.9	25
149	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
150	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
151	Electronic Structure of Disordered Alloys, Surfaces and Interfaces. , 1997, , .		401
152	Interlayer Exchange Coupling: Effect of Alloying. Acta Physica Polonica A, 1997, 91, 15-25.	0.5	2
153	Magnetic Properties. , 1997, , 225-257.		0
154	Numerical Implementation. , 1997, , 287-309.		0
155	Bulk Systems, Overlayers and Surfaces. , 1997, , 195-224.		0
156	Interlayer magnetic coupling: Effect of disorder in spacer. Journal of Magnetism and Magnetic Materials, 1996, 156, 245-246.	2.3	3
157	Evaluation of some basic positron-related characteristics of SiC. Physical Review B, 1996, 54, 2512-2517.	3.2	89
158	Interlayer magnetic coupling: Effect of interface roughness. Physical Review B, 1996, 53, 5125-5128.	3.2	78
159	Self-Consistent Greenâ€²s Function Method for Random Surfaces and Interfaces. NATO ASI Series Series B: Physics, 1996, , 237-264.	0.2	4
160	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
161	Positron Annihilation and MÃ¶ssbauer Spectroscopy in Highly Strained Fe₇₂Al₂₈ Alloy. Materials Science Forum, 1995, 175-178, 399-402.	0.3	3
162	Influence of the Crystal Potential on the Electron-Positron Momentum Density in 4sp and 3d Metals. Materials Science Forum, 1995, 175-178, 933-938.	0.3	0

#	Article	IF	Citations
163	Electron-Positron Interaction in Metallic Materials by Local Density Approach. Materials Science Forum, 1995, 175-178, 855-862.	0.3	2
164	Positron affinity for precipitates in reactor pressure vessel steels. Nuclear Engineering and Design, 1995, 158, 149-156.	1.7	29
165	Ferromagnetism of Imperfect Ultrathin Ru and Rh Films on a Ag(001) Substrate. Physical Review Letters, 1995, 74, 2551-2554.	7.8	47
166	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
167	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
168	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
169	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
170	Experimental And Theoretical Studies On The C15 Intermetallic Compounds MV2 (M=Zr, Hf AND Ta): Elasticity And Phase Stability. Materials Research Society Symposia Proceedings, 1994, 364, 1389.	0.1	2
171	Interatomic forces and atomic structure of grain boundaries in copper-bismuth alloys. Physical Review B, 1993, 47, 5571-5582.	3.2	86
172	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
173	The Influence of Crystal Potential and Positron Wave Function Anisotropy on the Momentum Density of Electron-Positron Pairs. Materials Science Forum, 1992, 105-110, 841-844.	0.3	2
174	A Comparative Atomistic Study of the Structure of Grain Boundaries in Tungsten. Materials Research Society Symposia Proceedings, 1992, 291, 491.	0.1	0
175	Tight-Binding Lmto Approach to the Electronic Structure and Atomic Configuration in Extended Defects in Metals. Materials Research Society Symposia Proceedings, 1992, 278, 205.	0.1	1
176	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
177	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
178	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
179	The Surface Green's Function in Semiconductors by the Tight-Binding Linear Muffin-Tin Orbital Method. Materials Research Society Symposia Proceedings, 1990, 209, 177.	0.1	1
180	Thermal vacancies and positron-lifetime measurements inFe76.3Al23.7. Physical Review B, 1990, 41, 11869-11874.	3.2	92

#	Article	IF	Citations
181	First-principles calculations of electronic structure in random hcp alloys: A Ru-Re example. Physical Review B, 1990, 41, 10459-10462.	3.2	6
182	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
183	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
184	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
185	Positron annihilation study of radiation damage in neutron-irradiated zirconium and its alloys. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 1989, 122, 243-249.	5.6	2
186	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
187	Relation between the strength characteristics of iron and nickel and the electronic structure of defects by positron annihilation spectroscopy. Physica Status Solidi A, 1988, 105, 357-363.	1.7	0
188	Electronic effects in the order-disorder transition in Î² brass. Journal of Physics F: Metal Physics, 1988, 18, 2387-2408.	1.6	9
189	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
190	A First-Principles Tight-Binding Method for Electronic Structure Calculations in Amorphous Solids*. Zeitschrift Fur Physikalische Chemie, 1988, 157, 515-520.	2.8	11
191	Spin-polarized positron annihilation and magnetic moment in Fe1â^'xCox alloys. Journal of Magnetism and Magnetic Materials, 1986, 62, 202-204.	2.3	6
192	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
193	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
194	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
195	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
196	Bonding and stability in the ordered alloys FeV and CoTi. Comparison with FeTi. Collection of Czechoslovak Chemical Communications, 1985, 50, 2093-2100.	1.0	0
197	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
198	Polarized Positron Annihilation and Enhancement Effects in Ferromagnetic Iron. Physica Status Solidi (B): Basic Research, 1984, 123, 649-652.	1.5	11

#	Article	IF	Citations
199	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
200	On bonding, stability and surface states in ordered alloys: FeTi and FeAl. Collection of Czechoslovak Chemical Communications, 1983, 48, 408-420.	1.0	1
201	Further band theory arguments elucidating the nature of the ordered state of the CsCl type alloy Î²'-CuZn. Collection of Czechoslovak Chemical Communications, 1983, 48, 2454-2463.	1.0	0
202	Positron annihilation in iron and B2-ordered alloys FeAl and FeTi. Journal of Physics F: Metal Physics, 1982, 12, 571-596.	1.6	43
203	The influence of a polymorphic transformation on positron annihilation in plastically deformed Ti-1.4 wt%Fe alloy. Physica Status Solidi A, 1980, 58, 645-650.	1.7	2
204	Positron annihilation in nonmetallic solids. Physics Letters, Section A: General, Atomic and Solid State Physics, 1979, 70, 47-48.	2.1	1
205	Positron annihilation in aluminium, subjected to the thermocyclic treatment. Physica Status Solidi A, 1979, 51, K113-K116.	1.7	0
206	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
207	Positron Annihilation in Some Uranium and Thorium Compounds. Physica Status Solidi (B): Basic Research, 1978, 89, K159.	1.5	2
208	Investigation of the surface of vanadium single crystals by positron annihilation. Physica Status Solidi (B): Basic Research, 1978, 90, K1.	1.5	3
209	Scalar fields around a charged, rotating black hole. European Physical Journal D, 1978, 28, 121-124.	0.4	3
210	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
211	Theory of strengthening of alpha titanium by interstitial solutes. European Physical Journal D, 1975, 25, 872-890.	0.4	28
212	Positron annihilation in some transition metal oxides. Physics Letters, Section A: General, Atomic and Solid State Physics, 1975, 53, 65-66.	2.1	3
213	Sessile Splittings of Screw Dislocations in H.C.P. Metals. Physica Status Solidi A, 1974, 24, K133-K136.	1.7	8
214	Transformation Paths in Transition-Metal Disilicides. Key Engineering Materials, 0, 465, 61-64.	0.4	0