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1151	Electronic structure and superconductivity in Pd-Ag-H and Pd-Rh-H alloys. <i>Physical Review B</i> , <b>1979</b> , 20, 177-183	3.3	46
1150	Theory of Auger relaxation energies in metals. <i>Physical Review B</i> , <b>1979</b> , 20, 1369-1376	3.3	120
1149	Moment-reversal calculation for bcc iron. <b>1980</b> , 79, 210-212		11
1148	Semiempirical calculation of the surface dipole barrier in metals. <b>1980</b> , 33, 59-62		12
1147	A theory of order-Disorder and antiphase domain boundary energies. <b>1980</b> , 11, 1747-1753		10
1146	On hybridizational gaps in energy band projections of some transition metal aluminides and CsAu and their stability. <b>1980</b> , 30, 593-596		2
1145	Electronic magnetic and cohesive properties of some nickel-aluminium compounds. <b>1980</b> , 10, 427-440		143
1144	The virial and Hellmann-Feynman theorems of an inhomogeneous electron gas. <b>1980</b> , 13, 3625-3637		14
1143	Self-consistent relativistic bandstructure for gold. <b>1980</b> , 10, 1135-1148		16
1142	Configuration of d holes in metals and alloys. <b>1980</b> , 10, L315-L320		21
1141	Electron density in simple metals. Relation to bulk and surface properties. <b>1980</b> , 10, 1995-2008		16
1140	Lattice Constant at the Insulator-Metal Transition of Crystalline Xenon. <b>1980</b> , 45, 933-935		29
1139	Prediction of solid solubility in alloys. <i>Physical Review B</i> , <b>1980</b> , 22, 5583-5589	3.3	68
1138	Pressure-induced structural transitions in partially ionic semiconductors: Self-consistent pseudopotential approach to ZnSe. <i>Physical Review B</i> , <b>1980</b> , 22, 4816-4824	3.3	36
1137	Optical properties and electronic structure of MiAl. <i>Physical Review B</i> , <b>1980</b> , 21, 5505-5510	3.3	20
1136	Microscopic Basis of Miedema's Empirical Theory of Transition-Metal Compound Formation. <b>1980</b> , 44, 429-433		134
1135	Spin-density functional calculations for chromium. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1980</b> , 20, 277-284	2.8	90

1134	First-principles calculations of the theoretical tensile strength of copper. <b>1980</b> , 41, 251-259		77
1133	Embedded cluster calculations for hydrogen chemisorption on the (111) surfaces of fcc Co, Ni, Cu, Rh, Pd and Ag. <b>1980</b> , 99, 609-630		40
1132	An ab initio pair potential applied to metals. <b>1980</b> , 41, 241-250		147
1131	Calculated magnetic moment of Emanganese. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1980</b> , 20, 107-110	2.8	48
1130	Chemical bonding and electronic structure of Pd2Si. <i>Physical Review B</i> , <b>1980</b> , 22, 4784-4790	3.3	172
1129	Validity of the frozen-core approximation and pseudopotential theory for cohesive energy calculations. <i>Physical Review B</i> , <b>1980</b> , 21, 2222-2228	3.3	89
1128	Magnetic moment of TiFe1©o from electronic structure calculations. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1980</b> , 15-18, 859-860	2.8	22
1127	Systematization of the stable crystal structure of all AB-type binary compounds: A pseudopotential orbital-radii approach. <i>Physical Review B</i> , <b>1980</b> , 22, 5839-5872	3.3	235
1126	Method for calculating wave functions in a nonspherical potential. <i>Physical Review B</i> , <b>1981</b> , 23, 6301-63	3063	33
1125	The quasi-binary cross section in the ternary system CuNiZn. <b>1981</b> , 15, 1362-1364		9
1125	The quasi-binary cross section in the ternary system CuNiZn. 1981, 15, 1362-1364  Self-consistent APW band structure calculations for the intermetallic compounds FeAl, CoAl, and NiAl. 1981, 112, 317-333		9
	Self-consistent APW band structure calculations for the intermetallic compounds FeAl, CoAl, and		
1124	Self-consistent APW band structure calculations for the intermetallic compounds FeAl, CoAl, and NiAl. <b>1981</b> , 112, 317-333		31
1124	Self-consistent APW band structure calculations for the intermetallic compounds FeAl, CoAl, and NiAl. 1981, 112, 317-333  Electronic States and Fermi Surface Properties of NiH. 1981, 103, 745-751		31
1124 1123 1122	Self-consistent APW band structure calculations for the intermetallic compounds FeAl, CoAl, and NiAl. 1981, 112, 317-333  Electronic States and Fermi Surface Properties of NiH. 1981, 103, 745-751  The magnetic properties of Ni3Al under high pressures. 1981, 106, 1-8		31 1 39
1124 1123 1122 1121 1120	Self-consistent APW band structure calculations for the intermetallic compounds FeAl, CoAl, and NiAl. 1981, 112, 317-333  Electronic States and Fermi Surface Properties of NiH. 1981, 103, 745-751  The magnetic properties of Ni3Al under high pressures. 1981, 106, 1-8  Solubility in nontransition homovalent alloys. Relation to the ionic radius. 1981, 103, 333-339		31 1 39 3
1124 1123 1122 1121 1120	Self-consistent APW band structure calculations for the intermetallic compounds FeAl, CoAl, and NiAl. 1981, 112, 317-333  Electronic States and Fermi Surface Properties of NiH. 1981, 103, 745-751  The magnetic properties of Ni3Al under high pressures. 1981, 106, 1-8  Solubility in nontransition homovalent alloys. Relation to the ionic radius. 1981, 103, 333-339  Magnetic moments of ferromagnetic and antiferromagnetic bcc and fcc iron. 1981, 81, 81-83  Self-consistent energy band calculations. 1981, 44, 139-212		31 1 39 3 196

1116	Experimental and theoretical band-structure studies of refractory metal silicides. <i>Physical Review B</i> , <b>1981</b> , 23, 2916-2922	3.3	121
1115	Virial theorem in the density-functional formalism: Forces in H2. <i>Physical Review B</i> , <b>1981</b> , 24, 6795-6800	3.3	56
1114	Electronic structure of amorphous transition-metal alloys. <i>Physical Review B</i> , <b>1981</b> , 23, 5176-5184	3.3	66
1113	The st transition in compressed lanthanum. <i>Physical Review B</i> , <b>1981</b> , 23, 5016-5029	3.3	87
1112	Volume dependence of magnetic hyperfine fields in Eu-intermetallic compounds. <i>Physical Review B</i> , <b>1981</b> , 23, 75-81	3.3	42
1111	Covalent magnetism: An alternative to the Stoner model. <b>1981</b> , 52, 2067-2069		108
1110	A comparison of melting point relations for metals, tetrahedral semiconductors, and metal carbides and nitrides with the rocksalt structure. <b>1981</b> , 52, 5547-5552		4
1109	Electronic structure of interstitial H in Cu. <b>1981</b> , 11, L287-L291		22
1108	Density functional-pseudopotential approach to the heat of formation in alloys of alkali metals. <b>1981</b> , 11, 2045-2053		15
1107	Structural morphology and electronic properties of the Si-Cr interface. <i>Physical Review B</i> , <b>1982</b> , 25, 498 <sup>-</sup>	1 <sub>3</sub> 4993	81
1106	Calculation of electronic structure of Pd on Nb(110) interface. <i>Physical Review B</i> , <b>1982</b> , 26, 7004-7007		17
		3.3	ĺ
1105	Electronic Structure Studies of CaxAl1⊠ Metallic Glasses. <b>1982</b> , 49, 575-578	3.3	49
1105	Electronic Structure Studies of CaxAl1\( \text{Metallic Glasses.} \) 1982, 49, 575-578  Self-consistent extended-muffin-tin orbital energy-band method: Application to LiC6. <i>Physical Review B</i> , 1982, 25, 4189-4195	3.3	,
	Self-consistent extended-muffin-tin orbital energy-band method: Application to LiC6. <i>Physical</i>		49
1104	Self-consistent extended-muffin-tin orbital energy-band method: Application to LiC6. <i>Physical Review B</i> , <b>1982</b> , 25, 4189-4195	3.3	49
1104	Self-consistent extended-muffin-tin orbital energy-band method: Application to LiC6. <i>Physical Review B</i> , <b>1982</b> , 25, 4189-4195  Band theory for the magnetic moment in the bcc Fe-Co alloy. <i>Physical Review B</i> , <b>1982</b> , 25, 3427-3429	3·3 3·3	49 23 30 25
1104 1103 1102	Self-consistent extended-muffin-tin orbital energy-band method: Application to LiC6. <i>Physical Review B</i> , <b>1982</b> , 25, 4189-4195  Band theory for the magnetic moment in the bcc Fe-Co alloy. <i>Physical Review B</i> , <b>1982</b> , 25, 3427-3429  Multiple-scattering approach to band theory. II. Fast band theory. <i>Physical Review B</i> , <b>1982</b> , 26, 1597-160	3·3 3·3	49 23 30 25

1098	Cohesion, Compound Formation and Phase Diagrams from First Principles. <i>Materials Research Society Symposia Proceedings</i> , <b>1982</b> , 19, 17		1
1097	Potentials in metals. <i>Lecture Notes in Physics</i> , <b>1982</b> , 115-129	0.8	2
1096	Magnetoacoustic oscillations and the Fermi surface of LaAg. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1982</b> , 28, 243-246	2.8	18
1095	Hydrides formed from intermetallic compounds of two transition metals: a special class of ternary alloys. <b>1982</b> , 45, 937-1039		324
1094	On the heats of formation of transition metal-p metal alloys. <b>1982</b> , 86, 181-186		40
1093	Theoretical studies of hydrogen interstitials in AB2 structure laves phase compounds. <b>1982</b> , 88, 231-23	7	14
1092	Covalent effects in the effective-medium theory of chemical binding: Hydrogen heats of solution in the 3d metals. <i>Physical Review B</i> , <b>1982</b> , 26, 2875-2885	3.3	390
1091	Ab initio calculation of the tetragonal shear moduli of the cubic transition metals. <i>Physical Review B</i> , <b>1982</b> , 26, 1527-1537	3.3	37
1090	Bond analysis of heats of formation: application to some group VIII and IB hydrides. <b>1982</b> , 12, 141-161		100
1089	Aspects of transition-metal magnetism. <b>1982</b> , 53, 2019-2023		93
1088	Electronic states and microstructure at the silicide-silicon interface. <b>1982</b> , 89, 433-446		38
1087	Quantitative determination of the pressure of He in bubbles in Al and Ni. <b>1982</b> , 44, 481-484		48
1086	Cellular theory of ordered AB alloys. <b>1982</b> , 44, 931-935		3
1085	Electronic structure of amorphous Zr based alloys with V, Cr and Mn studied by photoelectron spectroscopy and bandstructure calculations. <b>1982</b> , 44, 1551-1555		12
1084	Volume dependence of the spin-orbit splitting in the Au d-band. <b>1982</b> , 44, 51-54		10
1083	Ab-initio calculation of the heat of formation in the metallic transition metal monoxides. <b>1982</b> , 44, 339-	343	3
1082	Correlation between band structure and hydride formation in dilute palladium alloys. <b>1982</b> , 43, 697-70°	1	3
1081	Cellular density functional theory of the heat of formation of disordered simple alloys. <b>1982</b> , 114, 495-	501	3

Projected surface energy bands, Shockley surface states, stability and bonding in transition metal aluminides: The example of & CoAl. 1983, 33, 341-349

1079	New Class of Materials: Half-Metallic Ferromagnets. <b>1983</b> , 50, 2024-2027		3495
1078	Formation and coupling of magnetic moments in Heusler alloys. <i>Physical Review B</i> , <b>1983</b> , 28, 1745-1755	3.3	756
1077	Density-functional theory applied to phase transformations in transition-metal alloys. <i>Physical Review B</i> , <b>1983</b> , 27, 5169-5172	3.3	844
1076	The behaviour of hydrogen atoms implanted into metals. <b>1983</b> , 209-210, 773-790		73
1075	Self-consistent pseudopotential calculation of the electronic structure of PdH and Pd4H. <i>Physical Review B</i> , <b>1983</b> , 27, 3325-3337	3.3	82
1074	Iron-cobalt alloys: electronic and magnetic structure from SCF XASW cluster calculations. <b>1983</b> , 13, 311-	332	27
1073	Cluster approach to magnetic impurities in metals: Application to Mn, Mn, Mn, Fe and Fe. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1983</b> , 39, 295-308	2.8	15
1072	The density and pressure of helium in bubbles in metals. <b>1983</b> , 78, 315-325		61
1071	Atomistic studies of helium trapping in metals. <b>1983</b> , 78, 25-36		14
1070	Magnetism of amorphous metal-metal alloys. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1983</b> , 35, 192-198	2.8	98
1069	Theory of bonding of transition metals to nontransition metals. <i>Physical Review B</i> , <b>1983</b> , 27, 2005-2013	3.3	342
1068	Lattice-parameter dependence of ferromagnetism in bcc and fcc iron. <i>Physical Review B</i> , <b>1983</b> , 28, 5419-	- <b>5</b> <u>4</u> 322	188
1067	Theory of Invar and Heusler alloys. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1983</b> , 31-34, 88-94	2.8	71
1066	Weak itinerant ferromagnets: Ni3Al. <b>1983</b> , 13, L179-L183		48
1065	The electronic structure of non-stoichiometric Pd-rich Pd-Ag hydrides. <b>1983</b> , 13, 1869-1884		24
1064	Electronic structure of Ni and Pd alloys. I. X-ray photoelectron spectroscopy of the valence bands. <i>Physical Review B</i> , <b>1983</b> , 27, 2145-2178	3.3	295
1063	Split-Off Narrow d-Band States above EF in Transition-Metal Alloys. <b>1983</b> , 51, 1187-1190		50

1062	Electronic structure of transition-metal-transition-metal interfaces: Pd on Nb(110). <i>Physical Review B</i> , <b>1983</b> , 28, 3138-3149	3.3	43
1061	Stability in ordered and amorphous transition-metal compounds. <i>Physical Review B</i> , <b>1983</b> , 27, 7194-71983	3.3	78
1060	Generalized muffin-tin orbitals for electronic structure studies of surfaces, interfaces, and organic solids. <b>1983</b> , 78, 858-875		12
1059	Band theory of the magnetic interaction in MnO, MnS, and NiO. <i>Physical Review B</i> , <b>1983</b> , 28, 6443-6452	3.3	145
1058	Theoretical and experimental electronic structure of Zr-based transition-metal glasses containing Fe, Co, Ni, Cu, Rh, and Pd. <i>Physical Review B</i> , <b>1983</b> , 27, 2049-2054	3.3	126
1057	Density-functional study of interplanar binding in graphite. <i>Physical Review B</i> , <b>1983</b> , 27, 2458-2469	3.3	44
1056	Augmented Gaussian-orbital basis for atomic-cluster calculations within the density-functional formalism: Application to Cu2. <i>Physical Review B</i> , <b>1983</b> , 28, 5536-5548	3.3	43
1055	Magnetism in ordered and amorphous YCo3 and YFe3. <i>Physical Review B</i> , <b>1983</b> , 28, 5511-5514	3.3	25
1054	Band structure, cohesive properties, and Compton profile of Eland Eterium. <i>Physical Review B</i> , <b>1983</b> , 27, 3390-3405	3.3	52
1053	Calculation of electronic density of states for an amorphous Zr-Cu alloy. <i>Physical Review B</i> , <b>1983</b> , 28, 3753-3758	3.3	17
1052	Mixed states in RhA1, RhGa, and RhIn studied by photoemission spectroscopy and band-structure calculations. <i>Physical Review B</i> , <b>1983</b> , 28, 6774-6779	3.3	11
1051	Electron spectroscopy on metallic glasses. <b>1983</b> , 283-323		27
1050	Cohesive Properties of Alkali Halides and Simple Oxides in the Local-Density Formalism. <b>1983</b> , 52, 3506-3	513	54
1049	Relativistic diffraction theory: study of 3d and 4f surface ferromagnetism by polarised and unpolarised electrons. <b>1984</b> , 17, 5455-5471		12
1048	Alloying Effect on the Electronic Structure of Ni3Al ( []. <b>1984</b> , 53, 653-663		139
1047	Fully relativistic band structure of ferromagnetic Fe and Gd. <b>1984</b> , 14, L173-L178		33
1046	Transition-metal monoxides: Itinerant versus localized picture of superexchange. <b>1984</b> , 55, 2318-2320		18
1045	"Band-gap theory" of strong ferromagnetism: Application to concentrated crystalline and amorphous Fe- and Co-metalloid alloys. <i>Physical Review B</i> , <b>1984</b> , 29, 1620-1632	3.3	193

1044	Linear augmented-Slater-type-orbital method for electronic-structure calculations. <i>Physical Review B</i> , <b>1984</b> , 29, 2896-2904	3.3	75
1043	Energy-band analysis of ordered Fe and Co compounds: Implications for amorphous ferromagnets. <i>Physical Review B</i> , <b>1984</b> , 30, 6565-6572	3.3	17
1042	Transition between fundamental magnetic behaviors revealed by generalized SlaterPauling construction. <b>1984</b> , 55, 2353-2355		19
1041	Total energy and pressure in the Gaussian-orbitals technique. II. Pressure-induced crystallographic phase transition and equilibrium properties of aluminum. <i>Physical Review B</i> , <b>1984</b> , 29, 6434-6442	3.3	29
1040	Bonding in metal disilicides CaSi2 through NiSi2: Experiment and theory. <i>Physical Review B</i> , <b>1984</b> , 29, 3293-3302	3.3	151
1039	First-Principles Investigation of Metal-Hydrogen Interactions in NbH. <b>1984</b> , 53, 1586-1589		52
1038	Transition-Metal Monoxides: Band or Mott Insulators. <b>1984</b> , 52, 1830-1833		242
1037	Predicted Modifications in the Direct and Indirect Gaps of Tetrahedral Semiconductors. <b>1984</b> , 52, 675-6	78	59
1036	Electron charge density of alkali halides beyond the rigid-ion approximation. 1984, 49, 437-439		7
1035	Relativistic scattering calculations: On the study of surface magnetism by polarized and unpolarized electrons. <b>1984</b> , 49, 489-492		13
1034	X-ray absorption near edge structure of nickel hydride. <b>1984</b> , 51, 889-892		12
1033	Thermopower of mixed-valent CeNi5: instability vs band structure effects. <b>1984</b> , 51, 909-912		17
1032	Analytical wavefunction normalization procedure in KKR-method. <b>1984</b> , 53, 173-180		
1031	On the Electronic Structure of Palladium⊞ydrogen and Platinum⊞ydrogen Systems. <b>1984</b> , 121, 705-715	;	9
1030	Nonempirical methods in solid state theory. <b>1984</b> , 24, 501-517		1
1029	First principle theory of metallic magnetism. <b>1984</b> , 127, 257-263		65
1028	Ferromagnetism in some metallic vanadium compounds. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1984</b> , 45, 415-420	2.8	25
1027	Itinerant metamagnetism in YCO2. <b>1984</b> , 14, L129-L134		286

1026 Band-overl	ap metallization of BaS, BaSe, and BaTe. Physical Review B, 1984, 29, 5836-5839	3.3	58
Heat of for , 30, 4372-4	mation and band structure of binary and ternary metal hydrides. <i>Physical Review B</i> , <b>1984</b> 1381	3.3	118
1024 On the hyd	rogen site occupation in hydrides of intermetallics. <b>1984</b> , 103, 219-226		7
1023 X-ray absor	ption near-edge structure of metal hydrides. <b>1984</b> , 103, 337-347		18
1022 Self-consist	tent relativistic band structure of the noble metals. <b>1984</b> , 14, 97-112		286
1021 Properties	of SiO2 in a high-pressure fluorite structure phase. <b>1984</b> , 11, 617-619		10
	y of insulating transition-metal monoxides: Band-structure calculations. <i>Physical Review</i> , 4734-4747	3.3	522
1019 Electronic a	and magnetic structure of BCC Fe-Co alloys from band theory. <b>1984,</b> 14, 2659-2671		152
	nlung isochromat spectra and density-of-states calculations for the 3d and 4d transition usical Review B, <b>1984</b> , 30, 6921-6930	3.3	123
1017 Explicit, Fir	st-Principles Tight-Binding Theory. <b>1984</b> , 53, 2571-2574		2458
1016 Half-metall	ic ferromagnets and their magneto-optical properties (invited). <b>1984</b> , 55, 2151-2154		146
1015 Calculation	of Cohesive Energy of NaF. <b>1984</b> , 53, 3112-3119		4
	omparison of angle resolved photoemission spectra with calculated band structures of inpounds. <b>1985</b> , 459-464		6
	agnetic Phases with Total-Energy Spin-Polarized Band Calculations. <i>Materials Research</i> Apposia Proceedings, <b>1985</b> , 63, 117		3
1012 Binding me	chanism and itinerant magnetism of ZrFe2 and YFe2. <b>1985</b> , 130, 26-28		65
1011 The atomic	structure of alloy surfaces: Ni3Al{001}. <b>1985</b> , 53, 175-178		34
1010 Electronic s	structure of ferromagnetic Gd. <b>1985</b> , 53, 529-532		118
1009 <b>Equilibriu</b> m	properties of the cubic phases of cobalt. <b>1985</b> , 55, 971-975		63

1008	Embedded cluster model studies of impurities at metal surfaces. <b>1985</b> , 18, 59-188		23
1007	Spin and orbital moments in Upt3. <b>1985</b> , 54, 389-393		48
1006	The valence band structure of VMo solid solutions. <b>1985</b> , 58, 293-297		11
1005	Quadratic augmented plane wave method for self-consistent band structure calculations. <b>1985</b> , 35, 62-	71	6
1004	Exchange mechanisms in diluted magnetic semiconductors. <b>1985</b> , 56, 347-350		144
1003	Electron-phonon matrix element: Friedel sum rule and modified rigid-muffin-tin approximation. <b>1985</b> , 15, 2145-2156		3
1002	de Haas-van Alphen frequencies and upper critical field anisotropy in Nb3Sn. <b>1985</b> , 15, 297-316		17
1001	Spectroscopic ellipsometry of Ni3Al in comparison with band-structure calculations. <b>1985</b> , 15, 1195-120	1	18
1000	Band-reordering effects in the ultra-high-pressure equation of state of lithium. <b>1985</b> , 15, L247-L251		25
999	Angle-resolved photoelectron spectroscopy and band-structure calculations of CdI2. <i>Physical Review B</i> , <b>1985</b> , 31, 6739-6754	3.3	35
998	Self-consistent electronic-band-structure calculation for Hg3AsF6. <i>Physical Review B</i> , <b>1985</b> , 31, 2881-288	<b>85</b> .3	13
997	Comparison of optical reflectivity measurements, electron spectroscopy, and band-structure calculations of binary transition-metal alloys. <i>Physical Review B</i> , <b>1985</b> , 31, 7734-7738	3.3	4
996	Non-muffin-tin band theories of the multiple-scattering type. <i>Physical Review B</i> , <b>1985</b> , 32, 1339-1342	3.3	26
995	Zr1-xMoxN as a high-Tc superconductor. <i>Physical Review B</i> , <b>1985</b> , 32, 5489-5491	3.3	12
994	Simplified electrostatic model for band-gap underestimates in the local-density approximation. <i>Physical Review B</i> , <b>1985</b> , 31, 5178-5182	3.3	32
993	Electronic structure of LiZnN: Interstitial insertion rule. <i>Physical Review B</i> , <b>1985</b> , 32, 1386-1389	3.3	108
992	Linear augmented-Slater-type-orbital method for electronic-structure calculations. II. bcc, fcc, and hcp W. <i>Physical Review B</i> , <b>1985</b> , 32, 4876-4882	3.3	32
991	Zirconium nitride-a new material for Josephson junctions. <i>Physical Review B</i> , <b>1985</b> , 32, 8312-8316	3.3	84

990	Electronic structure of semiconducting beta -NaSn. <i>Physical Review B</i> , <b>1985</b> , 32, 2319-2325	3.3	47
989	Electronic structure of MnSb. <i>Physical Review B</i> , <b>1985</b> , 31, 1980-1996	3.3	95
988	New approach to minimal basis set with localized orbitals: Basic aspects and simple examples. <i>Physical Review B</i> , <b>1985</b> , 31, 2005-2013	3.3	10
987	Electronic structure of filled tetrahedral semiconductors. <i>Physical Review B</i> , <b>1985</b> , 31, 2570-2573	3.3	126
986	The electronic structure of MnBi. <b>1985</b> , 15, 2135-2144		86
985	Electronic structure calculations in liquid and amorphous metals. <b>1985</b> , 76, 147-156		2
984	The pseudopotential-density-functional method in momentum space: details and test cases. <b>1985</b> , 18, 4127-4142		29
983	L-edge x-ray-absorption systematics of the noble metals Rh, Pd, and Ag and the main-group metals In and Sn: A study of the unoccupied density of states in 4d elements. <i>Physical Review B</i> , <b>1985</b> , 31, 1888	3- <del>1</del> 902	129
982	Minimal basis sets in the linear muffin-tin orbital method: Application to the diamond-structure crystals C, Si, and Ge. <i>Physical Review B</i> , <b>1986</b> , 34, 2439-2449	3.3	397
981	Ferromagnetic phases of bcc and fcc Fe, Co, and Ni. <i>Physical Review B</i> , <b>1986</b> , 34, 1784-1791	3.3	649
980	Singular volume dependence of transition-metal magnetism. <b>1986</b> , 57, 2211-2214		197
979	Pressure dependence of the magnetisation of YFe2and ZrFe2: computation and experiment. <b>1986</b> , 16, L141-L144		40
978	Stability of metallic CsCl-structured alloys under ion irradiation. <b>1986</b> , 59, 4011-4016		19
977	Illustration of the linear-muffin-tin-orbital tight-binding representation: Compact orbitals and charge density in Si. <i>Physical Review B</i> , <b>1986</b> , 34, 5253-5269	3.3	708
976	Ab Initio Theory of the Ground State Properties of Ordered and Disordered Alloys and the Theory of Ordering Processes in Alloys. <i>Materials Research Society Symposia Proceedings</i> , <b>1986</b> , 81, 15		9
975	Effective-Pair-Interactions from Supercell Total Energy Calculations: Al-Transition Metal Alloys. <i>Materials Research Society Symposia Proceedings</i> , <b>1986</b> , 81, 39		
974	Intrinsically selective absorption in alloys of early with late transition metals. 1986, 14, 365-373		2
973	Magnetic and electronic properties of CuRh alloys. <b>1986</b> , 57, 103-107		8

972	Electronic structure of antistructure Co atoms and Co-vacancies in CoAl. 1986, 59, 429-432	9
971	Lithium equation-of-state at high pressure: Transition to statistical model behaviour. <b>1986</b> , 139-140, 364-366	2
970	Heat of formation of the ferromagnetic monohydride of Co. <b>1986</b> , 119, 234-236	2
969	Density functional pseudopotential calculation of the cohesive properties of Ordered (CsCl-Type) compounds of nontransition metals. <b>1986</b> , 133, 277-284	
968	Chemisorptive bonding of carbon monoxide on nickel (001): Formulation and application of a new pseudofunctional electron muffin tin approach. <b>1986</b> , 41, 61-73	17
967	FeMnSb: A half-metallic ferrimagnet. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1986</b> , 61, 330-336 2.8	72
966	Itinerant theory of localized magnetism. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1986</b> , 54-57, 603-60%	40
965	Total energy surfaces in the M-V plane for bcc and fcc cobalt. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1986</b> , 54-57, 955-956	65
964	Pressure dependence of the hyperfine field of YFe2 and ZrFe2. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1986</b> , 54-57, 1081-1082	34
963	Magnetic interactions in diluted magnetic semiconductors. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1986</b> , 54-57, 1283-1284	29
962	Recent developments in half-metallic magnetism. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1986</b> , 54-57, 1377-1380	170
961	Transport properties and electronic structure of nonmagnetic REAg compounds. <b>1986</b> , 64, 151-158	16
960	Quasiparticle band structure of CeCu2Si2 and CeAl3. <b>1986</b> , 65, 149-159	51
959	CrO2predicted as a half-metallic ferromagnet. <b>1986</b> , 16, L211-L215	581
958	Structure and dynamics of molten salts. <b>1986</b> , 49, 1001-1081	202
957	Temperature dependence of the electronic quasiparticle structure of ferromagnetic Gd <b>1986</b> , 60, 313-317	11
956	Differences between LaB6and CeB6by means of spectroscopic ellipsometry. <b>1986</b> , 16, 1617-1623	27
955	Near-Edge X-Ray Absorption Spectroscopy in Catalysis. <b>1986</b> , 203-296	44

954	Pseudofunction method: Application to a monolayer of CO and to the Si(111) surface. <i>Physical Review B</i> , <b>1986</b> , 34, 2656-2663	3.3	88
953	Total-energy calculations for intermetallic compounds with a first-principles linear combination of atomic orbitals method. <i>Physical Review B</i> , <b>1986</b> , 33, 747-754	3.3	21
952	Structural properties and electron density of NaCl. <i>Physical Review B</i> , <b>1986</b> , 33, 8629-8631	3.3	24
951	d-d transfer in transition-metal monoxides and dihalides. <i>Physical Review B</i> , <b>1986</b> , 33, 2733-2737	3.3	9
950	Calculated equation of state of InAs. <i>Physical Review B</i> , <b>1986</b> , 33, 5096-5098	3.3	15
949	Structural, electronic, and magnetic properties of Co: Evidence for magnetism-stabilizing structure. <i>Physical Review B</i> , <b>1986</b> , 33, 7852-7854	3.3	83
948	Elastic and magnetic interactions in a narrow twofold-degenerate band. <i>Physical Review B</i> , <b>1986</b> , 33, 5021-5027	3.3	13
947	Trends in hydrogen heats of solution and vacancy trapping energies in transition metals. <b>1986</b> , 16, 1161	1-1171	93
946	A Quantum-Mechanical Critique of the Miedema Rules for Alloy Formation. 1987, 40, 43-92		110
945	The electronic structure of glassy and crystalline Cu-Te alloys. <b>1987</b> , 20, 5233-5239		8
945 944	The electronic structure of glassy and crystalline Cu-Te alloys. <b>1987</b> , 20, 5233-5239  Band-structure calculations for Ni, Ni4H, Ni4H2, Ni4H3, and NiH. <i>Physical Review B</i> , <b>1987</b> , 35, 1993-2004	1 3.3	32
		<b>1</b> 3.3	
944	Band-structure calculations for Ni, Ni4H, Ni4H2, Ni4H3, and NiH. <i>Physical Review B</i> , <b>1987</b> , 35, 1993-2004	3.3	32
944	Band-structure calculations for Ni, Ni4H, Ni4H2, Ni4H3, and NiH. <i>Physical Review B</i> , <b>1987</b> , 35, 1993-2004.  Interatomic potentials in condensed matter via the maximum-entropy principle. <b>1987</b> , 59, 1108-1111.  Electronic theory of the alloy phase stability of Cu-Ag, Cu-Au, and Ag-Au systems. <i>Physical Review B</i> ,		32
944 943 942	Band-structure calculations for Ni, Ni4H, Ni4H2, Ni4H3, and NiH. <i>Physical Review B</i> , <b>1987</b> , 35, 1993-2004. Interatomic potentials in condensed matter via the maximum-entropy principle. <b>1987</b> , 59, 1108-1111  Electronic theory of the alloy phase stability of Cu-Ag, Cu-Au, and Ag-Au systems. <i>Physical Review B</i> , <b>1987</b> , 35, 2169-2173	3.3	32 11 136
944 943 942 941	Band-structure calculations for Ni, Ni4H, Ni4H2, Ni4H3, and NiH. <i>Physical Review B</i> , <b>1987</b> , 35, 1993-2004. Interatomic potentials in condensed matter via the maximum-entropy principle. <b>1987</b> , 59, 1108-1111. Electronic theory of the alloy phase stability of Cu-Ag, Cu-Au, and Ag-Au systems. <i>Physical Review B</i> , <b>1987</b> , 35, 2169-2173. Quasiparticle band structure of ferromagnetic EuS. <i>Physical Review B</i> , <b>1987</b> , 36, 5301-5305. Sodium chloride structural properties: Linearized augmented-plane-wave calculations and pressure	3-3	32 11 136
944 943 942 941 940	Band-structure calculations for Ni, Ni4H, Ni4H2, Ni4H3, and NiH. <i>Physical Review B</i> , <b>1987</b> , 35, 1993-2004. Interatomic potentials in condensed matter via the maximum-entropy principle. <b>1987</b> , 59, 1108-1111  Electronic theory of the alloy phase stability of Cu-Ag, Cu-Au, and Ag-Au systems. <i>Physical Review B</i> , <b>1987</b> , 35, 2169-2173  Quasiparticle band structure of ferromagnetic EuS. <i>Physical Review B</i> , <b>1987</b> , 36, 5301-5305  Sodium chloride structural properties: Linearized augmented-plane-wave calculations and pressure calibration. <i>Physical Review B</i> , <b>1987</b> , 35, 6395-6398  First-principles calculations of the phase diagrams of noble metals: Cu-Au, Cu-Ag, and Ag-Au.	3·3 3·3 3·3	32 11 136 11

936	Long-range order in AlxGa1-xAs. <i>Physical Review B</i> , <b>1987</b> , 36, 1526-1530	3.3	7
935	Dynamical corrections to density-functional theory for quasiparticles in ferromagnetic 4f systems. I. T=0 results for EuO. <i>Physical Review B</i> , <b>1987</b> , 35, 7015-7024	3.3	23
934	Real-space formulation of the mixed-basis pseudopotential method: Bulk structural properties of elemental copper. <i>Physical Review B</i> , <b>1987</b> , 35, 5457-5472	3.3	43
933	Effective-pair interactions in transition-metal alloys: A supercell total-energy approach. <i>Physical Review B</i> , <b>1987</b> , 35, 4858-4864	3.3	50
932	Method for calculating the electronic structures of large molecules; helical polymers. <b>1987</b> , 87, 7125-7	145	145
931	Optical absorption in TiNxOy-compounds. <b>1987</b> , 61, 4606-4611		28
930	Hydrogen in transition metals. <b>1987</b> , 146-163		1
929	Electronic Band Structure and Point-Contact Spectroscopy of the Organic Superconductor (BEDT-TTF)213. <b>1987</b> , 149-157		3
928	Linearized band structure methods. <b>1987</b> , 1-57		59
927	The Curie temperature of the ferromagnetic transition metals and their compounds. <b>1987</b> , 17, 2421-24	130	191
926	Electronic structure of MoSe2, MoS2, and WSe2. I. Band-structure calculations and photoelectron spectroscopy. <i>Physical Review B</i> , <b>1987</b> , 35, 6195-6202	3.3	451
925	Electronic structure and total energy calculations for transition metal hydrides. <b>1987</b> , 130, 249-259		32
924	The calculation of the electronic properties of the monohydride of cobalt by the linear muffin tin orbital method. <b>1987</b> , 130, 261-265		3
923	Photoemission study of the electronic structure of Zr-Pd compounds and their relation to hydride formation. <b>1987</b> , 130, 301-305		7
922	Electronic structure of some 3D transition-metal pyrites. <b>1987</b> , 20, 4135-4144		114
921	Band structure and chemical bonding in transition metal carbides and nitrides. <b>1987</b> , 13, 211-257		182
920	BANDSTRUCTURE OF HEAVY FERMIONS IN CeCu2Si2 AND CeAl3. 1987, 254-256		
919	Self-consistent band structure for E(BEDT TTF) 2 I 3. <b>1987</b> , 62, 801-805		58

918	Band theoretical studies of the electronic structure of oxides. <b>1987</b> , 14, 315-319	9
917	Electron and Positron States in Disordered Alloys. <b>1987</b> , 102, 31-46	9
916	Valence fluctuations in La2⊠SrxCuO4. <b>1987</b> , 63, 451-456	42
915	Symmetry breaking in La2-xBaxCuO4. <b>1987</b> , 64, 421-424	16
914	Potassium at high pressure: Anomaly in the 500 kbar-regime. <b>1987</b> , 62, 97-100	6
913	Ab inition determinations of oscillator strengths of metals and semiconductors from ASW. <b>1987</b> , 145, 5-15	2
912	Possibility of green light emission from GaP/AlP (001) superlattices. 1987, 37, 269-273	16
911	Electronic structure of NiAl. <b>1987</b> , 30, 599-603	
910	Electronic structure and bonding in metal hydrides, studied with photoelectron spectroscopy. <b>1987</b> , 66, 441-458	22
909	Electron-phonon interaction in LaAg. <b>1987</b> , 68, 291-298	22
908	Bandstructure of heavy fermions in CeCu 2 Si 2 and CeAl 3. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1987</b> , 63-64, 254-256	5
908		
	Materials, 1987, 63-64, 254-256  Theoretical study of TiO and Pb+ centers in alkali halide and alkaline earth fluoride type crystals.	
907	Materials, 1987, 63-64, 254-256  Theoretical study of TiO and Pb+ centers in alkali halide and alkaline earth fluoride type crystals. 1987, 35, 655-657  The influence of structural defects on the electronic properties of interstitial alloysIJ Lattice	5
907	Materials, 1987, 63-64, 254-256  Theoretical study of TiO and Pb+ centers in alkali halide and alkaline earth fluoride type crystals.  1987, 35, 655-657  The influence of structural defects on the electronic properties of interstitial alloys Lattice vacancies. 1988, 49, 465-477	5 40
907 906 905	Materials, 1987, 63-64, 254-256  Theoretical study of TiO and Pb+ centers in alkali halide and alkaline earth fluoride type crystals. 1987, 35, 655-657  The influence of structural defects on the electronic properties of interstitial alloys Lattice vacancies. 1988, 49, 465-477  First principles calculation of thermodynamic properties of noble-metal alloys. 1988, 36, 547-553	5 40
907 906 905 904	Materials, 1987, 63-64, 254-256  Theoretical study of TiO and Pb+ centers in alkali halide and alkaline earth fluoride type crystals. 1987, 35, 655-657  The influence of structural defects on the electronic properties of interstitial alloys Lattice vacancies. 1988, 49, 465-477  First principles calculation of thermodynamic properties of noble-metal alloys. 1988, 36, 547-553  Influence of structural vacancies on electronic state of interstitial phases. 1988, 29, 1-8  Optical Properties of (Zn, Mn) and (Cd, Mn) Chalcogenide Mixed Crystals and Superlattices. 1988,	5 40 55

900	X-ray photoelectron spectroscopy on amorphous CuxTe100₪ and NixTe100₪. <b>1988</b> , 99, 277-280		1
899	Optical reflectivity of glassy Pd?U?Si alloys. <b>1988</b> , 99, 313-316		4
898	Itinerant magnetism in K2NiF4-type compounds. <b>1988</b> , 153-155, 1237-1238		14
897	Understanding the formation of a heavy fermion ground state in UPt4Au. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1988</b> , 76-77, 91-92	2.8	9
896	Comparison of band-structure-calculation and ESR measurement of CePd3. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1988</b> , 76-77, 469-470	2.8	1
895	Heat of formation models. <b>1988</b> , 219-284		76
894	Calculated core hole effects on the K X-ray spectra of BCC transition metals. 1988, 72, 79-85		20
893	Magnetism in bcc and fcc manganese. <i>Physical Review B</i> , <b>1988</b> , 38, 423-432	3.3	64
892	Local-density-pseudofunction theory of bulk Si. <i>Physical Review B</i> , <b>1988</b> , 38, 2176-2178	3.3	19
891	Density functional theory of non-collinear magnetism. <b>1988</b> , 18, 469-483		266
890	Local spin-density functional theory of noncollinear magnetism (invited). <b>1988</b> , 63, 3482-3486		58
889	Theory of Heavy Fermion Systems. <b>1988</b> , 41, 1-150		248
888	Theory of exchange interactions and chemical trends in diluted magnetic semiconductors. <i>Physical Review B</i> , <b>1988</b> , 37, 4137-4154	3.3	332
887	Crystal and magnetic structures of ternary metal hydrides: A comprehensive review. <b>1988</b> , 87-138		46
886	Electronic properties. <b>1988</b> , 139-217		29
885	Heats of solution and lattice-expansion and trapping energies of hydrogen in transition metals. <i>Physical Review B</i> , <b>1988</b> , 38, 3690-3698	3.3	85
884	Calculated thermal properties of metals. <i>Physical Review B</i> , <b>1988</b> , 37, 790-799	3.3	682
883	Electronic structure of Cu2O and CuO. <i>Physical Review B</i> , <b>1988</b> , 38, 11322-11330	3.3	1318

882	Thin. <i>Physical Review B</i> , <b>1988</b> , 38, 3541-3544	3.3	18
881	Magnetism in bcc 3d transition metals: Onset and approach to the Hund's-rule limit. <i>Physical Review B</i> , <b>1988</b> , 38, 1613-1620	3.3	136
880	Coulomb correlation effects in the quasiparticle band structure of ferromagnetic rare-earth insulators. <i>Physical Review B</i> , <b>1988</b> , 37, 7663-7672	3.3	26
879	Magnetism of metastable phases: Band theory and epitaxy (invited). <b>1988</b> , 63, 4045-4050		66
878	Electronic structure of matter at high compression: Isostructural transitions and approach of the Fermi-gas limit. <i>Physical Review B</i> , <b>1988</b> , 37, 8674-8688	3.3	34
877	Magnetism, electronic structure, and Fermi surface of Ni3Al. <i>Physical Review B</i> , <b>1988</b> , 37, 6757-6762	3.3	64
876	Effect of bulk inversion asymmetry on. <i>Physical Review B</i> , <b>1988</b> , 37, 10923-10926	3.3	122
875	Magnetism in bcc 3d transition metals. <b>1988</b> , 64, 5598-5600		26
874	Electronic and structural properties of elemental copper: A pseudopotential-local-orbital calculation. <i>Physical Review B</i> , <b>1988</b> , 38, 7966-7971	3.3	41
873	Electronic structure and equation of state of compressed copper ASW calculation. 1988, 5, 193-196		1
872	The calculated electronic and structural properties of the transition-metal monoborides. <b>1988</b> , 21, 2829	9-2839	47
871	The calculated electronic and magnetic properties of the tetragonal transition-metal semi-borides. 1988, 21, 2841-2851		33
870	Transfer Integrals and Band Structures in (Et)2X Salts. <i>Materials Research Society Symposia Proceedings</i> , <b>1989</b> , 173, 119		
869	First-principles determination of the bulk phase diagram for body-centered-tetragonal copper: Application to epitaxial growth of Cu on Fe{100}. <i>Physical Review B</i> , <b>1989</b> , 39, 1575-1580	3.3	48
868	Origin of the difference in the magneto-optical Kerr effect between PtMnSb and NiMnSb. <i>Physical Review B</i> , <b>1989</b> , 40, 9318-9320	3.3	46
867	Spin-polarised relativistic electronic structure calculations. <b>1989</b> , 1, 8369-8383		54
866	Band structure, photoelectron spectroscopy, and transport properties of SnTaS2. <i>Physical Review B</i> , <b>1989</b> , 40, 12111-12125	3.3	14
865	Photoemission and inverse photoemission of transition-metal silicides. <i>Physical Review B</i> , <b>1989</b> , 39, 600	18369010	5 92

864	Magnetism in fcc rhodium and palladium. <i>Physical Review B</i> , <b>1989</b> , 39, 471-474	3.3	162
863	Electronic structure of the half-metallic ferromagnet KCrSe2. <i>Physical Review B</i> , <b>1989</b> , 40, 7973-7976	3.3	14
862	Cluster interactions and physical properties of Al-transition-metal alloys. <i>Physical Review B</i> , <b>1989</b> , 40, 912-923	3.3	44
861	Simple formula for the atomic forces in the augmented-plane-wave method. <i>Physical Review B</i> , <b>1989</b> , 40, 1560-1564	3.3	140
860	Electronic theory for phase stability of nine AB binary alloys, with A=Ni, Pd, or Pt and B=Cu, Ag, or Au. <i>Physical Review B</i> , <b>1989</b> , 39, 5792-5797	3.3	92
859	Applications of the quadratic Korringa-Kohn-Rostoker band-theory method. <i>Physical Review B</i> , <b>1989</b> , 39, 8187-8192	3.3	27
858	The effect of structural vacancies and substitutional impurities on the electronic and magnetic properties of cobalt, nickel, copper and palladium monohydrides. <b>1989</b> , 1, 9195-9208		
857	Full-potential linear augmented-Slater-type-orbital method. <i>Physical Review B</i> , <b>1989</b> , 40, 2757-2766	3.3	60
856	H-H interactions in Pd. <i>Physical Review B</i> , <b>1989</b> , 40, 1993-1996	3.3	41
855	Electronic theory for solid-solution hardening and softening of dilute Al-based alloys: Elastic-moduli enhancement of Al-Li alloys. <i>Physical Review B</i> , <b>1989</b> , 39, 7509-7516	3.3	32
854	Magnetovolume instabilities and ferromagnetism versus antiferromagnetism in bulk fcc iron and manganese. <i>Physical Review B</i> , <b>1989</b> , 39, 6957-6961	3.3	384
853	Electronic structure of metallic and semiconducting alkali-metal-lead compounds. <i>Physical Review B</i> , <b>1989</b> , 39, 8263-8274	3.3	37
852	Calculated electronic structure and magnetic properties of Y-Fe compounds. <i>Physical Review B</i> , <b>1989</b> , 39, 13072-13085	3.3	129
851	Electric fields and valence-band offsets in n+n. <i>Physical Review B</i> , <b>1989</b> , 40, 10402-10406	3.3	28
850	Band-structure calculations of Fe1/3TaS2and Mn1/3TaS2, and transport and magnetic properties of Fe0.28TaS2. <b>1989</b> , 1, 6363-6379		30
849	Pseudo-atom calculation of energetics in metals. <b>1989</b> , 1, 8359-8368		21
848	The electronic structure of NiAl and NiSi. <b>1989</b> , 1, 9131-9139		22
847	The electronic structure of 4d and 5d silicides. <b>1989</b> , 1, 9117-9129		25

846	Equation of state and electronic transfer for Al, Cu, Pb and Ta under ultrahigh pressures. <b>1989</b> , 138, 513-516	1
845	Temperature dependence of the electrical resistivity of REFe2 compounds. <b>1989</b> , 69, 1007-1010	14
844	Constrained total-energy calculations: Ferrimagnetism and antiferromagnetism in b.c.c. manganese. <b>1989</b> , 71, 203-206	22
843	Metastable magnetic ground-state of hcp-Fe. <b>1989</b> , 72, 631-633	43
842	Band structure calculations for magnetic and superconducting systems. <b>1989</b> , 159, 7-11	1
841	The Electronic Band Structure and Non-Empirical Calculations of Cohesive Properties of Refractory Compounds. <b>1989</b> , 151, 407-440	33
840	Unoccupied electronic states of CuO: An oxygen 1s x-ray-absorption spectroscopy investigation.  Physical Review B, 1989, 39, 4886-4890  3-3	84
839	Electronic structure of RhTi phases. <b>1989</b> , 147, 181-184	4
838	Heat of solution and site energies of hydrogen in disordered transition-metal alloys. <i>Physical Review B</i> , <b>1989</b> , 40, 1481-1494	31
837	The electronic structure of some monovalent-metal intercalates of TiS2. <b>1989</b> , 1, 4297-4309	33
836	Relative stability of LI2, DO22, and DO23 structures in MAl3 compounds. <b>1989</b> , 4, 1060-1063	118
835	Band-structure calculations, and magnetic and transport properties of ferromagnetic chromium tellurides (CrTe, Cr3Te4, Cr2Te3). <b>1989</b> , 1, 9141-9161	111
834	Ag2O band structure and x-ray-absorption near-edge spectra. <i>Physical Review B</i> , <b>1989</b> , 39, 9831-9838 3.3	55
833	Non-collinear itinerant magnetism: the case of Mn3Sn. <b>1989</b> , 1, 8155-8176	93
832	First-principles calculation of impurity-solution energies in Cu and Ni. <i>Physical Review B</i> , <b>1989</b> , 39, 930-9393	109
831	Design of High Elastic Modulus Alloy Using First Principles Electronic Theory. <i>Materials Research Society Symposia Proceedings</i> , <b>1990</b> , 186, 271	
830	AB Initio Calculations of Structural Energetics of Transition-Metal Aluminides and Silicides. <i>Materials Research Society Symposia Proceedings</i> , <b>1990</b> , 213, 19	1
829	Quantum-Mechanical Origins of Complex Structures in Al-Transition Metal Compounds. <i>Materials Research Society Symposia Proceedings</i> , <b>1990</b> , 186, 53	

828	Phase Stability and Role of Ternary Additions on Electronic and Mechanical Properties of Aluminum Intermetallics*. <i>Materials Research Society Symposia Proceedings</i> , <b>1990</b> , 213, 3		6
827	First-Principles Calculation of L10-Disorder Transition Temperature for Au–Pd Alloy. <b>1990</b> , 31, 315-316		9
826	Theory of electronic states in lattices and superlattices. <b>1990</b> , 13, 1-80		8
825	Electronic structure and bonding properties in TiSi2. <b>1990</b> , 78, 423-430		33
824	Magnetic and magneto-optical properties of NiMnSb1-xSnx compounds in relation to their electronic band structure. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1990</b> , 86, 326-332	2.8	7
823	Instability of diatomic deuterium in fcc palladium. <b>1990</b> , 9, 367-370		3
822	Structural phase transition of NaH and LiH under high pressure. <b>1990</b> , 143, 473-476		7
821	Antiferromagnetic and ferromagnetic gamma-manganese generalisation of the fixed-spin-moment method. <b>1990</b> , 161, 139-142		14
820	Magneto-volume effects in Fe-Ni invar: A first principles theory. <b>1990</b> , 161, 153-156		24
819	On the calculation of combined corrections in the LMTO method. <b>1990</b> , 88, 243-249		10
818	Stability of atomic and diatomic hydrogen in fcc palladium. <b>1990</b> , 73, 327-330		7
817	X-ray emission and absorption studies of silicides in relation to their electronic structure. <b>1990</b> , 41, 629	-633	23
816	Electronic structure and magnetism of transition-metal-stabilized YFe12-xMx intermetallic compounds. <i>Physical Review B</i> , <b>1990</b> , 41, 11790-11797	3.3	105
815	Cohesive, electronic, and structural properties of Al3Li: An important metastable phase. <i>Physical Review B</i> , <b>1990</b> , 41, 12432-12440	3.3	22
814	Ab initio band-structure calculation of the semiconductor FeSi2. <b>1990</b> , 68, 3027-3029		89
813	Calculated optical properties of approximate structures for incommensurately modulated calaverite. <b>1990</b> , 105, 125-130		
812	Electronic structure of NiAl. <i>Physical Review B</i> , <b>1990</b> , 42, 1582-1597	3.3	123
811	Absence of volume metastability in bcc copper. <i>Physical Review B</i> , <b>1990</b> , 41, 2699-2703	3.3	37

## (1991-1990)

810	Highly symmetric Mn sites in icosahedral Ti-Mn. <i>Physical Review B</i> , <b>1990</b> , 41, 1695-1698	3.3	21
809	Antiferromagnetism in 4d transition metals. <i>Physical Review B</i> , <b>1990</b> , 42, 10322-10328	3.3	23
808	Critical structure in the density of states from non-atom-centered Wannier functions. <i>Physical Review B</i> , <b>1990</b> , 41, 9803-9813	3.3	4
807	Bands versus bonds in electronic-structure theory of metal oxides: Application to luminescence of copper in zinc oxide. <i>Physical Review B</i> , <b>1990</b> , 42, 1423-1430	3.3	43
806	Augmented-plane-wave forces. <i>Physical Review B</i> , <b>1990</b> , 42, 9728-9731	3.3	122
805	Core-hole effects in the x-ray-absorption spectra of transition-metal silicides. <i>Physical Review B</i> , <b>1990</b> , 41, 11899-11910	3.3	77
804	Valence-electron contributions to the electric-field gradient in hcp metals and at Gd nuclei in intermetallic compounds with the ThCr2Si2 structure. <i>Physical Review B</i> , <b>1990</b> , 42, 4645-4655	3.3	139
803	Relativistic effects on ground state properties of 4d and 5d transition metals. <b>1990</b> , 2, 4371-4394		139
802	First-principles electronic structure calculations for incommensurately modulated calaverite. <b>1990</b> , 2, 4829-4847		16
801	Antiferromagnetism in 3d transition metals. <i>Physical Review B</i> , <b>1990</b> , 42, 8361-8366	3.3	88
800	Ab initio electronic-structure calculations on the Nb/Zr multilayer system. <i>Physical Review B</i> , <b>1990</b> , 41, 5613-5626	3.3	69
799	Theory of magnetic superlattices: Interlayer exchange coupling and magnetoresistance of transition metal structures (invited). <b>1990</b> , 67, 5914-5919		155
798	First-principles study of short range order and instabilities in AuCu, AuAg and AuPd alloys. <b>1991</b> , 39, 493	3-501	48
797	First-principles calculation of the Ag-Cu phase diagram. <i>Physical Review B</i> , <b>1991</b> , 44, 5411-5418	3.3	122
796	Precise density-functional method for periodic structures. <i>Physical Review B</i> , <b>1991</b> , 44, 7888-7903	3.3	391
795	The electronic structure of ordered binary Co-Pt compounds. <b>1991</b> , 3, 1133-1152		54
794	Itinerant magnetism and electronic properties of FeGe2. <b>1991</b> , 3, 7199-7208		9
793	Self-consistently determined properties of solids without band-structure calculations. <i>Physical Review B</i> , <b>1991</b> , 44, 8454-8458	3.3	344

792	First-principles statistical mechanics of structural stability of intermetallic compounds. <i>Physical Review B</i> , <b>1991</b> , 44, 512-544	3.3	274
791	Calculation of hyperfine fields in binary Y-Fe compounds and in Y2Fe14B. <b>1991</b> , 69, 6222-6224		36
790	Long and Short Range Oscillatory Exchange Coupling in Fe/Cu and Co/Cu Magnetic Multilayers. <i>Materials Research Society Symposia Proceedings</i> , <b>1991</b> , 231, 195		18
789	Experiences with the Quadratic Korringa-Kohn-Rostoker Band Theory Method. <i>Materials Research Society Symposia Proceedings</i> , <b>1991</b> , 253, 27		1
788	Local-spin-density calculations of antiferromagnetic YBa2Cu3O6 and La2CuO4. <b>1991</b> , 77, 45-48		6
787	Systematics in the electronic structure of amorphous transition metal/tin alloys. <b>1991</b> , 133, 107-110		1
786	A new approach to a non-local density functional for the calculation of electron correlation energies. <b>1991</b> , 172, 27-30		
7 <sup>8</sup> 5	Half-metallic magnetism in the 1990s. <b>1991</b> , 172, 45-50		84
784	Spin waves and Heisenberg exchange constants for ∃ron. <b>1991</b> , 172, 79-84		11
783	Full-potential LMTO calculations for atomic relaxations at semiconductor-semiconductor interfaces. <b>1991</b> , 172, 175-183		57
782	First principles band structure calculations for rare earth-transition metal compounds: magnetization, hyperfine parameters and magnetocrystalline anistropy. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1991</b> , 99, 55-70	2.8	96
781	The electronic and magnetic properties of NiFe3N. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1991</b> , 101, 251-252	2.8	8
780	Lattice spacing dependence of the magnetization of the nitride Mn4N. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1991</b> , 101, 419-420	2.8	8
779	Electronic Structure and Interlayer Exchange Coupling in Fe/Cr Superlattices. <b>1991</b> , 15, 875-880		28
778	Heterojunction band offsets and effective masses in III-V quaternary alloys. <b>1991</b> , 6, 27-31		376
777	Electronic structure and stability of palladiumhydrogen (deuterium) systems, PdH(D)n, 1 <b>5B. 1991</b> , 172-174, 1363-1370		10
776	Electronic Structure. <b>1991</b> , 1-126		
775	Energetics of C11b, C40, C54, and C49 structures in transition-metal disilicides. <b>1991</b> , 6, 1512-1517		35

774	Ab initio electronic-structure calculations on the Nb/Cu multilayer system. 1991, 3, 7651-7662		4
773	Band structures of non-collinear magnets in gamma -Mn and gamma -Fe. <b>1991</b> , 3, 8665-8682		6
77 <sup>2</sup>	Ab initio electron-structure calculations on the Nb/Ta multilayer system. <b>1991</b> , 3, 3945-3957		3
771	First-principles electronic structure and optical properties of CrSi2. <i>Physical Review B</i> , <b>1991</b> , 44, 9042-90	<b>4</b> 43	31
770	Theoretical study of the structural stability of CuPd and CuPt alloys: Pressure-induced phase transition of CuPt alloy. <i>Physical Review B</i> , <b>1991</b> , 43, 947-955	3.3	7
769	X-ray-emission studies of chemical bonding in transition-metal silicides. <i>Physical Review B</i> , <b>1991</b> , 44, 819	5 <del>,.</del> §20	349
768	Multiple-scattering theory and the quadratic Korringa-Kohn-Rostoker method. <i>Physical Review B</i> , <b>1991</b> , 44, 8467-8472	3.3	4
767	Magnetic and metal-insulator transitions in metallic hydrogen. <i>Physical Review B</i> , <b>1991</b> , 43, 825-832	3.3	2
766	Relative stability of the Al12W structure in Al-transition-metal compounds. <i>Physical Review B</i> , <b>1991</b> , 43, 12176-12186	3.3	22
765	Bands versus bonds in sulfides: Theoretical investigation of the luminescence of copper in zinc sulfide. <i>Physical Review B</i> , <b>1991</b> , 43, 14188-14195	3.3	12
764	Valence-electron contributions to the electric-field gradient and the crystal field at rare-earth sites in intermetallic compounds. <b>1991</b> , 69, 5590-5592		78
763	Total energies of improved quasicrystal models. <b>1991</b> , 67, 3128-3131		13
762	Relativistic spin-polarized calculation of the electronic structure of antiferromagnetic chromium. <b>1992</b> , 4, 7555-7564		3
761	The electrical resistivities of liquid Pd-Bi alloys and the band structure of crystalline beta -PdBi2and PdBi. <b>1992</b> , 4, 2389-2395		11
760	A method for the calculation of spin susceptibilities of itinerant systems for finite temperature. <b>1992</b> , 4, 8097-8104		7
759	Cohesive properties, electronic structure, and bonding characteristics of RuAlA comparison to NiAl. <b>1992</b> , 7, 592-604		51
758	First-principles calculation of the magnetocrystalline anisotropy energy of the pnictide MnSb. <b>1992</b> , 4, 10469-10478		6
757	Static nonuniform magnetic susceptibility of selected transition metals. <b>1992</b> , 4, 6927-6942		34

756	Ab initio electronic-structure calculations on the Au/Ag multilayer system and Au epitaxy on the Ag(110) surface. <i>Physical Review B</i> , <b>1992</b> , 45, 4469-4478	3.3	7
755	Ab initio calculation of local magnetic moments and the crystal field in scrR2Fe14B (scrR=Gd, Tb, Dy, Ho, and Er). <i>Physical Review B</i> , <b>1992</b> , 45, 3161-3163	3.3	38
754	Band-theory description of high-energy spectroscopy and the electronic structure of LiCoO2. <i>Physical Review B</i> , <b>1992</b> , 46, 3729-3735	3.3	103
753	Total energies and magnetic moments in Fe, V, and ordered FeV. <i>Physical Review B</i> , <b>1992</b> , 45, 2934-293	83.3	23
75 <sup>2</sup>	Ferrimagnetic-antiferromagnetic phase transition in Mn2-xCrxSb: Electronic structure and electrical and magnetic properties. <i>Physical Review B</i> , <b>1992</b> , 45, 5395-5405	3.3	66
75 <sup>1</sup>	Applications of the quadratic Korringa-Kohn-Rostoker band-theory method to complex lattices. <i>Physical Review B</i> , <b>1992</b> , 45, 1425-1427	3.3	2
75 <sup>0</sup>	Band structures of nonmagnetic transition-metal oxides: PdO and PtO. <i>Physical Review B</i> , <b>1992</b> , 46, 424	163 <u>4</u> 249	9 36
749	Antiferromagnetic-ferromagnetic transition in FeRh. <i>Physical Review B</i> , <b>1992</b> , 46, 2864-2873	3.3	146
748	Electronic structure of SnS deduced from photoelectron spectra and band-structure calculations. <i>Physical Review B</i> , <b>1992</b> , 46, 7363-7373	3.3	101
747	Electronic structure of antistructure defects in FeAl. <b>1992</b> , 4, 1905-1914		10
746	Pressure dependence of the magnetization of NiFe3N. <b>1992</b> , 8, 455-457		
746 745	Pressure dependence of the magnetization of NiFe3N. <b>1992</b> , 8, 455-457  Quasi-particles in heavy fermion systems. <b>1992</b> , 41, 203-302		159
			159
745	Quasi-particles in heavy fermion systems. <b>1992</b> , 41, 203-302  Theoretical Investigation on the Luminescence Transition Probabilities in the Phosphor ZnO:Cu.		
745 744	Quasi-particles in heavy fermion systems. <b>1992</b> , 41, 203-302  Theoretical Investigation on the Luminescence Transition Probabilities in the Phosphor ZnO:Cu. <b>1992</b> , 96, 1765-1770  Correlation between the Electrostatic Potential and the Occupation of Interstitial Sites by		3
745 744 743	Quasi-particles in heavy fermion systems. 1992, 41, 203-302  Theoretical Investigation on the Luminescence Transition Probabilities in the Phosphor ZnO:Cu. 1992, 96, 1765-1770  Correlation between the Electrostatic Potential and the Occupation of Interstitial Sites by Hydrogen in Metallic Systems. 1992, 96, 1639-1645  Ein Verfahren zur Berechnung der temperaturabhägigen Suszeptibilitälitineranter Systeme aus	3.3	3
745 744 743 742	Quasi-particles in heavy fermion systems. 1992, 41, 203-302  Theoretical Investigation on the Luminescence Transition Probabilities in the Phosphor ZnO:Cu. 1992, 96, 1765-1770  Correlation between the Electrostatic Potential and the Occupation of Interstitial Sites by Hydrogen in Metallic Systems. 1992, 96, 1639-1645  Ein Verfahren zur Berechnung der temperaturabhägigen Suszeptibilitälitineranter Systeme aus Grundzustandsgrän. 1992, 96, 1708-1711	3.3	3

738	Ab initio calculated magneto-optical Kerr effect of ferromagnetic metals: Fe and Ni. <i>Physical Review B</i> , <b>1992</b> , 45, 10924-10933	3.3	230
737	Calculated electronic and magnetic structure of the nitrides NiFe3N and PdFe3N. <i>Physical Review B</i> , <b>1992</b> , 45, 4000-4007	3.3	89
736	Electronic structure and optical properties of europium-activated yttrium oxide phosphor. <i>Physical Review B</i> , <b>1992</b> , 45, 10902-10906	3.3	123
735	Development of the quadratic Korringa <b>K</b> ohn <b>R</b> ostoker band theory method. <b>1992</b> , 42, 1025-1035		
734	Temperature variation of the electron density of states in bcc iron. <b>1992</b> , 83, 559-562		4
733	Electronic structure and properties of the superconductor Pb2SrxLa2\(\mathbb{R}\)Cu2O6+\(\mathbb{I}\)1992, 201, 119-125		5
732	Electronic structure of the layered compounds K[SnSb], K[SnAs] and Sr[Sn2As2]. <b>1992</b> , 97, 93-104		20
731	The magnetic properties of iron nitride: Fe8N. <b>1992</b> , 87, 91-96		38
730	Calculated electronic and magnetic structure of UNi2Al3 and UPd2Al3. 1992, 87, 299-304		30
729	Electronic structure of epitaxial interfaces. <b>1992</b> , 38, 545-639		12
728	Ab initio investigation of microscopic enhancement factors in tuning the magneto-optical Kerr effect. <b>1992</b> , 88, 309-315		79
727	Electronic and magnetic states of Fe. Journal of Magnetism and Magnetic Materials, 1992, 103, 314-324	2.8	129
726	Calculated electronic band structure and magnetic moments of ferrites. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1992</b> , 103, 212-220	2.8	131
725	A critical discussion of some models for the concentration dependence of magnetic moments in amorphous and microcrystalline alloys of Fe, Co or Ni with P. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1992</b> , 117, 45-60	2.8	17
724	Noncollinear spiral magnetic order in itinerant-electron magnets. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1992</b> , 104-107, 695-696	2.8	8
723	Magnetovolume effects in PtFe3N. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1992</b> , 104-107, 1927-1	928	11
722	M <b>B</b> auer-Spektroskopie und Elektronenstrukturberechnungen an Nitridoferraten(III): Li3[FeN2] und Ba3[FeN3]. <b>1992</b> , 104, 1632-1634		7

720	ASW first principles calculation of the intrinsic and extrinsic stacking fault energies in aluminum. <b>1993</b> , 174, 437-440	6
719	Calculated electronic structure of SnFe3N. <b>1993</b> , 85, 273-279	31
718	Correlations between the structural distortion of LaCuO3 lattice and the resulting physical properties. <b>1993</b> , 85, 961-965	16
717	A comparative study of electronic structure of alkaline earth sulfides as hosts for phosphors. <b>1993</b> , 18, 214-219	5
716	Ab initio electron theory for hard-magnetic rare-earth-transition-metal intermetallics. <b>1993</b> , 57, 67-76	46
715	First principles calculations of the hyperfine field at Gd nuclei in intermetallic compounds. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1993</b> , 118, 175-181	32
714	Temperature-dependent bandstructure of ferromagnetic metals with localized moments. <b>1993</b> , 90, 413-425	11
713	Isomer-shift of interstitial and substitutional iron in silicon and germanium. <b>1993</b> , 92, 155-162	31
712	A study of ionic solids by means of new density-functional theory techniques. <b>1993</b> , 15, 243-251	5
711	Pd-Ti bimetallics: A study of the electronic structure using x-ray photoelectron spectroscopy and x-ray-absorption near-edge structure. <i>Physical Review B</i> , <b>1993</b> , 48, 7836-7840	36
710	Transition metal silicides in silicon technology. <b>1993</b> , 56, 1397-1467	158
709	Atomic mobilities on a stepped Cu(100) surface. <b>1993</b> , 287-288, 881-885	24
708	Wave function imaging of the PbS(001) surface with scanning tunneling microscopy. <b>1993</b> , 287-288, 1106-111	18
707	Theory of bonding in transition-metal carbides and nitrides. <i>Physical Review B</i> , <b>1993</b> , 48, 11685-11691 3.3	346
706	Supercell calculations for transition metal impurities in palladium. <b>1993</b> , 5, 5099-5112	21
705	Cohesive properties and electronic structure of 5d-transition-metal carbides and nitrides in the NaCl structure. <i>Physical Review B</i> , <b>1993</b> , 48, 11673-11684	75
704	Trends in bulk moduli from first-principles total-energy calculations. <i>Physical Review B</i> , <b>1993</b> , 48, 7665-7667	25
703	Calculations of systematics in B2 structure 3d transition metal aluminides. <b>1993</b> , 197, 229-242	41

First-principles calculations of the instability leading to the Invar effect. Physical Review B, 1993, 47, 8706:\$720142 702 Local Magnetic Moments of Conduction Electrons in Gadolinium. 1993, 23, 661-666 701 32 Electronic structure, itinerant magnetism and orbital ordering of K2NiF4-type compounds. 1993, 5, 2987-3002 20 700 Chapter 2 Energy band theory of metallic magnetism in the elements. 1993, 7, 97-137 699 First-principles calculation of heats of formation for Au-Cu, Au-Pd and Au-Ag alloys with thermal 698 25 vibration effects. 1993, 5, 1473-1480 Resistivities and band structures of alkaline-earth-pnictide systems. 1993, 5, 7551-7562 697 15 696 The gap in YH3and its lattice structure. 1993, 5, 4805-4816 45 On the stability of random and intermetallic phases of LiAl alloys. 1993, 5, 851-860 695 Oxygen 1s x-ray absorption of tetravalent titanium oxides: A comparison with single-particle 694 3.3 243 calculations. Physical Review B, 1993, 48, 2074-2080 Constant-volume pair potential for Al-transition-metal compounds. Physical Review B, 1993, 47, 2961-2969. 693 13 Microscopic theory of the martensitic transition in Fe1-xNix. Physical Review B, 1993, 47, 5589-5596 692 3.3 35 . **1993**, 29, 3249-3251 691 690 Local magnetic moments in bcc Co. Physical Review B, 1993, 47, 5854-5860 3.3 15 Interband optical properties of Ni3Al. Physical Review B, 1993, 48, 16974-16978 689 80 3.3 Electronic And Magnetic Properties Of Copper-containing Chromium Sulfospinel: A first-principles 688 Study.. 1993, 687 Local susceptibilities in the paramagnetic regime of Y(Fe,Al)2. 1993, 5, 7277-7288 Agneto-Optical Spectra of Copt3: Experiments and First Principles Calculations. Materials Research 686 9 Society Symposia Proceedings, 1993, 313, 501 A calculation of the temperature-dependent susceptibility of Pd and dilute Pd1-xAgxand 685 6 PdHxalloys. **1994**, 6, 2603-2618

684	Cohesive and electronic properties of ordered Li-Al intermetallic compounds. <b>1994</b> , 6, 3389-3402		15
683	Band-structure and cluster-model calculations of LaCoO3 in the low-spin phase. <i>Physical Review B</i> , <b>1994</b> , 49, 7210-7218	3.3	95
682	Physics of the Be(0001) surface core-level spectrum. <i>Physical Review B</i> , <b>1994</b> , 50, 17480-17486	3.3	20
681	A new ferromagnetic oxide La2MnIrO6: Synthesis, characterization, and calculation of its electronic structure. <b>1994</b> , 75, 4617-4620		23
680	Magnetic and electronic structure of CoH. <i>Physical Review B</i> , <b>1994</b> , 49, 12801-12804	3.3	6
679	Spin fluctuations in gamma -Fe and in Fe3Pt Invar from local-density-functional calculations. <i>Physical Review B</i> , <b>1994</b> , 50, 291-301	3.3	148
678	Electronic structure and optical properties of FeSi, a strongly correlated insulator. <i>Physical Review B</i> , <b>1994</b> , 49, 2219-2222	3.3	106
677	Theory for itinerant electrons in noncollinear and incommensurate structured magnets (invited). <b>1994</b> , 76, 6694-6699		9
676	Electronic-structure-based pair potentials for aluminum-rich cobalt compounds. <i>Physical Review B</i> , <b>1994</b> , 49, 9322-9330	3.3	44
675	Two-center overlap integrals over Slater-type orbitals constrained to a spherical integration volume: Analytical expressions. <b>1994</b> , 50, 2232-2238		3
674	Magnetic polarization of the Pd spacer and interlayer magnetic couplings in Fe/Pd (001) superlattices: First principles calculations. <i>Physical Review B</i> , <b>1994</b> , 49, 299-309	3.3	44
673	Magnetism of UT2Si2 (T=Cr,Mn,Fe,Co,Ni,Cu,Ru,Rh,Pd,Os) from spin-density-functional calculations. <i>Physical Review B</i> , <b>1994</b> , 50, 9258-9264	3.3	29
672	One-dimensional ordering of In atoms in a Cu(100) surface. <i>Physical Review B</i> , <b>1994</b> , 49, 4871-4880	3.3	7
671	Ab initio study of the interlayer magnetic couplings in Fe/Pd(001) superlattices and of the polarization induced in the Fe and Pd layers. <b>1994</b> , 75, 6467-6469		13
670	Electronic structure of superconducting LuNi2B2C, YPd2B2C and related intermetallic compounds. <b>1994</b> , 228, 331-335		98
669	X-ray absorption and dichroism of transition metals and their compounds. <b>1994</b> , 67, 529-622		553
668	Inferred physical properties of UT2Si2 (T = Ru, Rh, Pd) from spin-density functional calculations. <b>1994</b> , 91, 183-186		24
667	Temperature-dependent electronic structure of gadolinium. <b>1994</b> , 94, 409-421		47

## (1995-1994)

666	Investigation of the magnetic structure of CrN. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1994</b> , 134, 34-40	2.8	18
665	Magneto-optical and magnetic properties of some solid solutions of C1b-Heusler compounds. Journal of Magnetism and Magnetic Materials, <b>1994</b> , 130, 247-254	2.8	17
664	Magnetic and electronic structure of the nitrides PdFe3N and MnFe3N. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1994</b> , 130, 353-362	2.8	34
663	Band theoretical investigations within the local density approximation of the ferromagnetic silicides: UFe10Si2, UCo10Si2 and YFe10Si2. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1994</b> , 137, 293-304	2.8	16
662	Clusters and bulk beryllium: A molecular orbital versus crystal orbital study. <b>1994</b> , 44, 897-904		1
661	High field MBsbauer investigations of FexN (x=3,4). <b>1994</b> , 94, 2093-2097		3
660	The chemical bonding and electronic properties of metal borides. <b>1994</b> , 63, 711-734		30
659	A theoretical study of the magneto-optical Kerr effect in FeX (X=Co,Ni,Pd,Pt). <b>1994</b> , 6, 285-292		38
658	Ag L-edge x-ray-absorption near-edge-structure study of charge redistribution at the Ag site in Au-Ag alloys. <i>Physical Review B</i> , <b>1994</b> , 49, 13776-13779	3.3	31
657	The electronic structure of magnetic transition metallic materials. <b>1994</b> , 57, 1289-1344		58
656	Computer applications to materials science and engineering emphasized on the Japanese point of view. <b>1994</b> , 2, 103-110		
655	Local-density functional and on-site correlations: The electronic structure of La2CuO4 and LaCuO3. <i>Physical Review B</i> , <b>1994</b> , 49, 14211-14228	3.3	577
654	The electronic and magnetic structures of alpha - and beta -manganese. <b>1994</b> , 6, 6557-6564		32
653	Electronic structure, magnetic, and Fermi-surface properties of UPd2Al3. <i>Physical Review B</i> , <b>1994</b> , 50, 15834-15842	3.3	48
652	Local Electronic Structure and Cohesion of Grain Boundaries in Ni3Al. <i>Materials Research Society Symposia Proceedings</i> , <b>1994</b> , 364, 743		1
651	Calculated magneto-optical properties of metallic compounds. <b>1995</b> , 56, 1529-1533		5
650	Theoretical investigation of cross luminescence in CdF2. <b>1995</b> , 24, 347-350		2
649	The electronic structure of ZrO2: Band structure calculations compared to electron and x-ray spectra. <b>1995</b> , 93, 659-665		32

648	Theory of the giant magneto-optical Kerr effect in MnPt3 and PtMnSb. <b>1995</b> , 94, 255-259		39
647	Magnetic and electronic structure of Fe/Pd (0 0 1) monolayers. <b>1995</b> , 95, 537-542		11
646	Magnetism in the Huesler alloys: Co2TiSn and Co2TiAl. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1995</b> , 140-144, 183-184	2.8	46
645	High field M\(\mathbb{B}\)sbauer spectroscopy on Mn-substituted Fe3N. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1995</b> , 140-144, 117-118	2.8	4
644	The calculated electronic and magnetic properties of U2T2Sn (T?Fe, Co, Ni). <i>Journal of Magnetism and Magnetic Materials</i> , <b>1995</b> , 151, 263-272	2.8	25
643	Relation between interfacial magnetism and spin-dependent scattering at non-ideal Fe/Cr and Fe/V interfaces. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1995</b> , 151, 341-353	2.8	63
642	Orbital magnetism in URhSn. Journal of Magnetism and Magnetic Materials, 1995, 140-144, 1389-1390	2.8	6
641	Cohesive, electronic and magnetic properties of the transition metal aluminides FeAl CoAl and NiAl. <b>1995</b> , 7, 6019-6034		58
640	Electronic structure of the misfit-layer compound (SnS)1.17NbS2 deduced from band-structure calculations and photoelectron spectra. <i>Physical Review B</i> , <b>1995</b> , 52, 2336-2347	3.3	50
639	Oscillatory magnetism in compounds of iron with 4d metals. <i>Physical Review B</i> , <b>1995</b> , 52, 3448-3452	3.3	19
638	Relativistic calculations of the magneto-optical Kerr spectra in (001) and (111) US, USe, and UTe. <i>Physical Review B</i> , <b>1995</b> , 52, 3561-3570	3.3	72
637	Electric-field-gradient calculations on cadmium in cadmium-helium vacancy clusters in tungsten. <i>Physical Review B</i> , <b>1995</b> , 52, 3909-3916	3.3	3
636	The Electronic Structure of La 2 BaCuO 5: A Magnetic Insulator. <b>1995</b> , 31, 385-391		35
635	Structure and magnetism of epitaxially strained Pd(001) films on Fe(001): Experiment and theory. <i>Physical Review B</i> , <b>1995</b> , 51, 6364-6378	3.3	84
634	Electronic structure of beta -PbO2 and its relation with BaPbO3. <i>Physical Review B</i> , <b>1995</b> , 52, 11740-117	<b>43</b> 3	31
633	Spin polarization of Mn layers on Fe(001). <i>Physical Review B</i> , <b>1995</b> , 52, 10127-10135	3.3	31
632	Chapter II Theory of surface structure and bonding. <b>1995</b> , 4, 63-119		2
631	Reconstruction of the true wavefunctions from the pseudowavefunctions in a crystal and calculation of electric field gradients. <b>1995</b> , 7, 9201-9217		39

630	Physics and Control of Conduction Type in \$bf CuInS_{2}\$ with Defect Chalcopyrite Structure. <b>1995</b> , 34, L1584-L1587		15
629	Magnetic structures of uranium compounds: Effects of relativity and symmetry. <b>1995</b> , 75, 946-949		61
628	Electronic structure of the lead monoxides: Band-structure calculations and photoelectron spectra. <i>Physical Review B</i> , <b>1995</b> , 52, 11690-11697	3.3	80
627	Electronic structure of antimony-doped tin oxide. <i>Physical Review B</i> , <b>1995</b> , 51, 13972-13976	3.3	111
626	Ab initio study of the structural properties of LiF, NaF, KF, LiCl, NaCl, and KCl. <i>Physical Review B</i> , <b>1995</b> , 51, 3391-3396	3.3	99
625	An analysis of the zero differential overlap approximation. Towards an improved semiempirical MO method beyond it. <b>1995</b> , 92, 13-47		9
624	A first-principles study of exchange integrals in magnetite. <b>1995</b> , 7, 4227-4237		39
623	Initial- and final-state effects in the conduction bands of 2H-MoS2(0001) studied by k  -resolved inverse photoemission spectroscopy. <i>Physical Review B</i> , <b>1995</b> , 52, 12095-12101	3.3	19
622	Incommensurate crystal structures. <b>1995</b> , 4, 79-202		179
621	Investigation of the electronic structure of carbon-containing TiAl. <b>1996</b> , 233, 112-120		7
620	Ab-initio study of structural stability and magnetism of Ni2CuSn. <b>1996</b> , 4, 335-338		6
619	Band-theoretical description of the magneto-optical spectra of UAsSe. <i>Physical Review B</i> , <b>1996</b> , 53, R10	)4 <u>3</u> .7-R	10,440
618	Electronic structure of intercalated metal disulfides ( and ) studied by XPS and theoretical calculations. <b>1996</b> , 245, 30-39		36
617	Band theory for electronic and magnetic properties of. <b>1996</b> , 8, 983-989		69
616	Exchange-Coupled Spin-Fluctuation Theory: Application to Fe, Co, and Ni. <b>1996</b> , 77, 334-337		168
615	Calculated magneto-optical properties of pure and doped MnBi. <b>1996</b> , 8, 8681-8694		21
614	Band Structure Calculations of Ferromagnetic Chromium Tellurides CrSiTe3and CrGeTe3. <b>1996</b> , 100, 5863-5867		64
613	FIRST-PRINCIPLES THEORY AND PREDICTIONS OF THE KERR EFFECT. <i>Journal of the Magnetics Society of Japan</i> , <b>1996</b> , 20, S1_47-52		9

612	Electronic Structures of P-Type Doped CuInS2. <i>Materials Research Society Symposia Proceedings</i> , <b>1996</b> , 426, 201		7
611	A New Phase of Cu <b>B</b> t Alloy <b>T</b> heoretical Prediction and Experimental Support. <b>1996</b> , 65, 2178-2181		3
610	Color of pure and alkali-doped cerium sulfide: A local-density-functional study. <i>Physical Review B</i> , <b>1996</b> , 54, 2428-2435	3	52
609	Improved analysis of hyperfine fields in Fe, Co and Ni, and application to orbital magnetism in intermetallic compounds. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1996</b> , 159, 55-63	8	20
608	(Fe,Mn) Si: Transitions from a magnetic to a nonmagnetic state and from metallic to semiconducting behaviour. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1996</b> , 157-158, 715-716	8	8
607	Theoretical study of high-TC molecular-based cyanide magnets. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1996</b> , 157-158, 417-418	8	6
606	Quasi two-dimensional magnetism in MnGaGe. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1996</b> , 157-158, 721-722	8	О
605	Structure, chemistry and bonding at grain boundaries in Ni3All The role of boron in ductilizing grain boundaries. <b>1996</b> , 44, 1637-1645		61
604	Noncollinear magnetic order and electronic properties of U2Pd2Sn and U3P4. <b>1996</b> , 217, 167-180		22
603	Crystal structure and band structure calculations of Pb13TaS2 and Sn13NbS2. <b>1996</b> , 226, 259-267		11
602	Energy-band theory of the magneto-optical Kerr effect of selected ferromagnetic materials. <b>1996</b> , 29-47		10
601	First-principles LSDF study of weak ferromagnetism in Fe 2 O 3. <b>1996</b> , 33, 447-452		40
600	The origins of the similarities between late transition metals and early transition metal monocarbides. <b>1996</b> , 107-120		5
599	First-principles theoretical study of metallic states of DCNQI-(Cu,Ag,Li) systems. <i>Physical Review B</i> , <b>1996</b> , 54, 10452-10464	3	53
598	Type-II antiferromagnetism in compounds of iron with 4d metals. <i>Physical Review B</i> , <b>1996</b> , 54, 11933-1193	<b>5</b>	6
597	First-principles study of the giant magneto-optical Kerr effect in MnBi and related compounds. <b>1996</b> , 80, 1099-1105		47
596	Calculated magneto-optical Kerr spectra of compounds (X = V, Cr, Mn, Fe and Co). <b>1996</b> , 8, 5769-5780		36
595	P-Type Doping of the Group V Elements in CulnS\$_{bf 2}\$. <b>1996</b> , 35, L1562-L1565		15

594	The Fermi surface of. <b>1996</b> , 8, 901-909	50
593	Electronic structure of the misfit layer compound : band structure calculations and photoelectron spectra. <b>1996</b> , 8, 1663-1676	22
592	Electronic structure of the misfit layer compound: band-structure calculations and photoelectron spectra. <b>1996</b> , 8, 5367-5382	14
591	Electronic Structures and Effects of S Substitutions in \$bf CuIn(S_{0.875}X_{0.125})_{2}~(X=O,,N,,P,,C,,Si,or,B)\$. <b>1996</b> , 35, L370-L373	4
590	Electronic and magnetic properties of UPdSn: the itinerant 5f electrons approach. <b>1997</b> , 9, 4897-4908	9
589	Magnetic order and chemical bonding in the high-TC molecule-based cyanide magnets CsM[Cr(CN)6] (M=Mn, Ni) from first principles. <i>Physical Review B</i> , <b>1997</b> , 56, 8959-8969	24
588	Many-body definition of a Fermi surface: Application to angle-resolved photoemission. <i>Physical Review B</i> , <b>1997</b> , 55, 13473-13478	60
587	TiFe1☑ Coxsalloys and the influence of antistructural atoms. <i>Physical Review B</i> , <b>1997</b> , 55, 16110-16121 3.3	9
586	Ab initio analysis of magnetic properties in noncollinearly ordered Mn4N. <i>Physical Review B</i> , <b>1997</b> , 55, 2995-3002	28
585	Electronic Structures and Host Excitation of LaPO4, La2O3, and AlPO4. <b>1997</b> , 12, 2183-2190	27
584	Materials Design for the Fabrication of Low-Resistivity p-Type GaN Using a Codoping Method. <b>1997</b> , 36, L180-L183	95
583	Exchange-coupled spin-fluctuation theory: calculation of magneto-elastic properties. <b>1997</b> , 9, 7885-7902	13
582	Control of Valence States by a Codoping Method in P-Type GaN Materials. <i>Materials Research Society Symposia Proceedings</i> , <b>1997</b> , 468, 105	4
581	Electronic properties and magnetic structure of U3X4 (X=P,As,Sb). <i>Physical Review B</i> , <b>1997</b> , 55, 11395-11 <del>4</del> .94	30
580	Recent Developments in Multiple Scattering Theory and Density Functional Theory for Molecules and Solids. <b>1997</b> , 1-58	
579	Full charge-density scheme with a kinetic-energy correction: Application to ground-state properties of the 4d metals. <i>Physical Review B</i> , <b>1997</b> , 55, 13521-13527	89
578	Theoretical investigations of the elastic constants in Laves phases. <b>1997</b> , 5, 449-465	60
577	Ordered compounds and magnetic properties of metallic multilayers. <b>1997</b> , 8, 182-191	3

576	Calculations of electronic and magnetic structures in ultra-thin magnetic systems. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1997</b> , 165, 62-69	2.8	13
575	Chemical bonding and magnetism in the equiatomic intermetallic system UCoSn from first principles. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1997</b> , 166, 321-328	2.8	9
574	Theoretical study of non-collinear magnetic orders in (FexCo1🛭)/Mnn superlattices. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1997</b> , 165, 450-453	2.8	9
573	Chemical bonding and magnetism in the ternary germanides UT2Ge2 (T = 3d transition metal) from local spin density functional calculations. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1997</b> , 174, 219-	2 <del>3</del> 5 <sup>8</sup>	13
572	Calculations of electronic and magnetic structures in ultra-thin magnetic systems. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1997</b> , 168, 62-69	2.8	6
571	NEXAFS investigations of transition metal oxides, nitrides, carbides, sulfides and other interstitial compounds. <b>1997</b> , 30, 1-152		492
570	Computational methods in the theory of chemical bonding in solids. 1997, 38, 459-482		1
569	Radially dependent antishielding factor (r) of the Sc3+ ion in the solid state. 1997, 49, 301-308		
568	Control of valence states by a codoping method in CuInS2. <b>1997</b> , 49, 391-397		6
567	Theory of the optical and magneto-optical spectra of cerium and uranium compounds. <b>1997</b> , 230-232, 544-549		18
566	Exchange-coupled spin-fluctuation theory: Application to Fe, Co and Ni. 1997, 237-238, 496-498		3
565	Calculated magneto-optical properties of pure and doped MnBi. <b>1997</b> , 237-238, 402-406		7
564	Calculation of theoretical strength of solids by linear muffin-tin orbitals (LMTO) method. <b>1997</b> , 234-236, 370-372		46
563	Electronic structure of intercalated metal disulfide () studied by XPS and theoretical calculations. <b>1997</b> , 87, 19-30		8
562	The electronic structure of the mixed valence compound Pb3O4. <b>1997</b> , 58, 561-566		34
561	The electronic structure of TiN and VN: X-ray and electron spectra compared to band structure calculations. <b>1997</b> , 102, 291-296		33
560	Spin-glass precursors in b.c.cmanganese. <b>1997</b> , 102, 729-733		18
559	Ab initio molecular dynamics calculations to study catalysis. <b>1997</b> , 61, 369-380		29

558	Local density functional calculations of the electronic structures of the intermetallic systems U2Fe2Sn and UFe2Ge2. <b>1997</b> , 61, 705-709		9
557	Electronic structures of p-type GaN codoped with Be or Mg as the acceptors and Si or O as the donor codopants. <b>1998</b> , 189-190, 532-536		18
556	Magnetic susceptibility and proton Knight shift in Pd-Ag and Pd-(rare earth) solid solution alloy hydrides. <b>1998</b> , 102, 629-641		2
555	Electronic structures and nature of host excitation in borates. <b>1998</b> , 102, 1772-1782		30
554	Electronic structure and magnetic properties of 2Fe/Pd and 2Pd/Fe multilayers. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1998</b> , 184, 293-301	2.8	10
553	Calculated magnetic and electronic properties of the double perovskites La2TIrO6 (T=Mn, Fe, Co). Journal of Magnetism and Magnetic Materials, <b>1998</b> , 187, 201-209	2.8	16
552	Magneto-optical spectroscopy in the valence-band energy regime: relationship to the magnetocrystalline anisotropy. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1998</b> , 188, 275-285	2.8	54
551	Magnetism of UT2Si2 compounds: Effect of the orbital polarization correction. <b>1998</b> , 106, 115-119		19
550	Optical properties of U3P4. <b>1998</b> , 253, 222-237		4
549	Ab initio study of the chemical role of carbon within TiAl alloy system: Application to composite materials. <b>1998</b> , 10, 314-318		6
548	Magnetic properties simulations of CoRu interfaces. <b>1998</b> , 10, 269-272		3
547	Optical and magneto-optical spectroscopy of uranium and plutonium compounds: recent theoretical progress. <b>1998</b> , 271-273, 831-836		14
546	Local spin density functional investigations of the ternary systems UT2Ge2 (T=Mn,Fe). <b>1998</b> , 275-277, 468-471		2
545	Magnetic order and defect structure of FexAl1⊠ alloys around x=0.5: An experimental and theoretical study. <i>Physical Review B</i> , <b>1998</b> , 58, 14922-14933	3.3	93
544	A Periodic Density Functional Theory and Hartreeflock Study of Alkali Halides with Gaussian Orbitals. <b>1998</b> , 102, 10310-10317		9
543	Electronic structure of V2O5: Role of octahedral deformations. <i>Physical Review B</i> , <b>1998</b> , 57, 12727-127	3₹.3	214
542	Electronic structure of FeS2: The crucial role of electron-lattice interaction. <i>Physical Review B</i> , <b>1998</b> , 57, 6350-6359	3.3	99
541	Electronic structure and total energy of transition metals from an spd tight-binding method: Application to surfaces and clusters of Rh. <i>Physical Review B</i> , <b>1998</b> , 58, 9721-9731	3.3	49

540	Role ofn-Type Codopants on Enhancingp-Type Dopants Incorporation inp-Type Codoped Znse. <i>Materials Research Society Symposia Proceedings</i> , <b>1998</b> , 510, 67		4
539	Intermetallic borocarbides: electronic structure, chemical bonding, and properties. <b>1998</b> , 67, 357-374		9
538	Role of Cl or I Codoping in Li-Doping Enhancement in ZnSe. <b>1998</b> , 37, L910-L912		13
537	Spin ordering in Fe3-x Mn x Si Heusler alloys. <b>1998</b> , 78, 629-636		22
536	Effects of Na Incorporation in p-Type CulnS2. <b>1998</b> , 37, L1478-L1480		13
535	The mechanism of antiferromagnetism in chromium. <b>1998</b> , 10, 6541-6552		24
534	EELS investigation of the electron conduction-band states in wurtzite AlN and oxygen-doped AlN(O). <i>Physical Review B</i> , <b>1998</b> , 58, 5106-5115	3.3	35
533	The conduction bands of MgO, MgS and. <b>1998</b> , 10, 10241-10248		38
532	The magnetic phases of face-centred-cubic iron. <b>1999</b> , 11, 5709-5715		11
531	Bandstructure calculations of the hexagonal and cubic phases of. <b>1999</b> , 11, 759-766		12
530	Ab initiomolecular dynamics in an all-electron mixed-basis approach: application to atomic insertions to C60. <b>1999</b> , 7, 621-630		20
529	Host Excitation and Luminescence in Large Band Gap Oxides. <i>Materials Research Society Symposia Proceedings</i> , <b>1999</b> , 560, 323		3
528	Theoretical study of the magnetism within Gd/Mo and Gd/W multilayers. <i>Physical Review B</i> , <b>1999</b> , 60, 10233-10241	3.3	4
527	Magnetic structure in ordered FeCr. <i>Physical Review B</i> , <b>1999</b> , 60, 56-59	3.3	9
526	Solution Using a Codoping Method to Unipolarity for the Fabrication of p-Type ZnO. <b>1999</b> , 38, L166-L10	59	511
525	Electronic properties of UX3 (X=Ga, Al, and Sn) compounds in high magnetic fields: Transport, specific heat, magnetization, and quantum oscillations. <i>Physical Review B</i> , <b>1999</b> , 59, 14473-14483	3.3	45
524	Ab initio calculation of the torques acting on localized magnetic moments including incomplete-basis-set corrections. <i>Physical Review B</i> , <b>1999</b> , 59, 13965-13972	3.3	7
523	Magnetic and electronic structure of Fe/Cu bilayers. <b>1999</b> , 350, 186-191		5

522	Effects of oxygen incorporation in p-type AlN crystals doped with carbon species. <b>1999</b> , 273-274, 113-1	15	21
521	Differences in the electronic structure and compensation mechanism between n-type Zn- and Cd-doped CuInS2 crystals. <b>1999</b> , 273-274, 927-929		15
520	Heterogeneous catalysis: looking forward with molecular simulation. <b>1999</b> , 50, 451-477		18
519	Electronic structure and activation energy of hydrogen in NEG alloy using nonlinear response theory. <b>1999</b> , 52, 333-340		
518	The Fe4N system revisited: an ab initio calculation study of the magnetic interactions. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1999</b> , 191, 234-240	2.8	58
517	High-temperature coercivity and Kerr spectroscopy on MnBi/Al multilayers. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1999</b> , 198-199, 131-133	2.8	1
516	Temperature-dependent quasiparticle bandstructure of ferromagnetic gadolinium. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1999</b> , 192, 529-542	2.8	27
515	Stress-induced ferrimagnetic orders in Fe/Ir multilayers. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1999</b> , 198-199, 306-308	2.8	2
514	Full-potential nonorthogonal local-orbital minimum-basis band-structure scheme. <i>Physical Review B</i> , <b>1999</b> , 59, 1743-1757	3.3	1478
513	Electrical properties of half-metallic PtMnSb-based Heusler alloys.		
512	Ab Initio Methods. <b>1999</b> , 7-138		5
511	Electronic structure and magnetic interactions in LiV 2 O 4. <b>1999</b> , 46, 762-767		59
510	Theory of the Anisotropic Magneto-Optical Kerr Effect in Artificial FeAu and MnAu and in XAu4 (X=V, Cr, Mn) Compounds. <i>Journal of the Magnetics Society of Japan</i> , <b>1999</b> , 23, S1_21-26		5
509	Control of Valence States in ZnO by Codoping Method. <i>Materials Research Society Symposia Proceedings</i> , <b>2000</b> , 623, 223		14
508	Materials Design for the Low-Resistivity in p-Type ZnO and Transparent Ferromagnet With Transition Metal Atom Doped ZnO: Prediction vs. Experiment. <i>Materials Research Society Symposia Proceedings</i> , <b>2000</b> , 623, 65		1
507	Local spin density functional investigations of the chemical bonding and of the magnetism in some uranium ternary intermetallic systems: How physics and chemistry can meet in the solid state. <b>2000</b> , 77, 911-926		4
506	Basic notions and applications of the augmented spherical wave method. <b>2000</b> , 77, 1007-1031		132
505	Band Magnetism in A2T2Sn (A=Ce, U; T=Ni, Pd) from Local Spin Density Functional Calculations. <b>2000</b> , 149, 449-454		30

504	Unipolarity of ZnO with a wide-band gap and its solution using codoping method. <b>2000</b> , 214-215, 552-55	5	101
503	Magnetic ordering in MnB2: an ab initio study. <b>2000</b> , 113, 509-512		10
502	Eude ab initio des structures lectroniques et magnEiques des systlmes YFe 2 et YFe 2 H 3 au sein de la thBrie de la fonctionnelle de la densit[(DFT). <b>2000</b> , 3, 27-33		4
501	Influence of incorporation of Na on p-type CuInS2 thin films. <b>2000</b> , 159-160, 345-349		10
500	Materials design of n-type CuInS2 thin films using Zn or Cd species. <b>2000</b> , 159-160, 350-354		13
499	Theoretical aspects of hyperfine interactions. <b>2000</b> , 128, 67-78		4
498	Understanding iron and its alloys from first principles. <b>2000</b> , 80, 141-153		16
497	Control of Defects in CuinS2 Thin Films by Incorporation of Na and O. <b>2000</b> , 39, L1280-L1282		12
496	Optical properties of itinerant UGa3: Ellipsometric measurements and first-principles theory. <i>Physical Review B</i> , <b>2000</b> , 61, 7415-7420	3.3	5
495	Electronic band structure of the layered compound TdWTe2. Physical Review B, 2000, 62, 10812-10823	3.3	82
494	Electronic structure of plutonium monochalcogenides. <i>Physical Review B</i> , <b>2000</b> , 61, 12825-12834	3.3	49
493	spd tight-binding model of magnetism in transition metals: Application to Rh and Pd clusters and slabs. <i>Physical Review B</i> , <b>2000</b> , 61, 7781-7794	3.3	85
492	Electronic structure, hydrogen site occupation and phase stability of Ti3Al upon hydrogenation. <b>2000</b> , 305, 35-42		11
491	Noncollinear magnetic order in U3Bi4. <b>2000</b> , 309, 31-38		10
490	The electronic structures of uranium borides from local spin density functional calculations. <b>2000</b> , 2, 43-51		13
489	Local spin density investigations in oxide systems with half metallic ferromagnetic properties. <b>2000</b> , 2, 523-532		6
488	Embedded Peierls instability and the electronic structure of MoO2. <b>2000</b> , 12, 4923-4946		76
487	The order of the magnetic phase transitions in RCo2(R = rare earth) intermetallic compounds. <b>2000</b> , 12, 9453-9464		92

486	From ASA Towards the Full Potential. <b>1999</b> , 85-114		30
485	Electronic structure of Na3Sb and Na2KSb. <i>Physical Review B</i> , <b>2000</b> , 61, 10035-10039	3.3	22
484	Phase stability and electronic structure of the HfAl3 compound. <i>Physical Review B</i> , <b>2001</b> , 64,	3.3	21
483	Electronic structure, bonding, and ground-state properties of AlB2-type transition-metal diborides. <i>Physical Review B</i> , <b>2001</b> , 63,	3.3	375
482	Electron localization on dislocations in metals: Real-space first-principles calculations. <i>Physical Review B</i> , <b>2001</b> , 64,	3.3	8
481	Investigation of the bonding and magnetic properties of U3Cu4Ge4 and structurally related systems. <b>2001</b> , 3, 227-232		
480	Phase stability and electronic structure in ZrAl3 compound. 2001, 319, 154-161		44
479	Theoretical investigation on site preference of foreign atoms in rare-earth intermetallics. <b>2001</b> , 319, 62-73		16
478	Density functional prediction of a magnetic ground state of UFeSi. <b>2001</b> , 321, 10-16		4
477	Sign reversal of the orbital moment via ligand states. <i>Physical Review B</i> , <b>2001</b> , 63,	3.3	32
477 476	Sign reversal of the orbital moment via ligand states. <i>Physical Review B</i> , <b>2001</b> , 63,  Codoping method for the fabrication of low-resistivity wide band-gap semiconductors in p-type GaN, p-type AlN and n-type diamond: prediction versus experiment. <b>2001</b> , 13, 8901-8914	3.3	32 97
	Codoping method for the fabrication of low-resistivity wide band-gap semiconductors in p-type	3.3	
476	Codoping method for the fabrication of low-resistivity wide band-gap semiconductors in p-type GaN, p-type AlN and n-type diamond: prediction versus experiment. <b>2001</b> , 13, 8901-8914  Electronic Structures and Nature of Host Excitation in Gallates. <i>Materials Research Society Symposia</i>	3.3	
476 475	Codoping method for the fabrication of low-resistivity wide band-gap semiconductors in p-type GaN, p-type AlN and n-type diamond: prediction versus experiment. <b>2001</b> , 13, 8901-8914  Electronic Structures and Nature of Host Excitation in Gallates. <i>Materials Research Society Symposia Proceedings</i> , <b>2001</b> , 667, 1	3.3	97
476 475 474	Codoping method for the fabrication of low-resistivity wide band-gap semiconductors in p-type GaN, p-type AlN and n-type diamond: prediction versus experiment. <b>2001</b> , 13, 8901-8914  Electronic Structures and Nature of Host Excitation in Gallates. <i>Materials Research Society Symposia Proceedings</i> , <b>2001</b> , 667, 1  Computation vs knowledge in materials innovation. <b>2001</b> , 4, 209-215	3.3	97
476 475 474 473	Codoping method for the fabrication of low-resistivity wide band-gap semiconductors in p-type GaN, p-type AlN and n-type diamond: prediction versus experiment. <b>2001</b> , 13, 8901-8914  Electronic Structures and Nature of Host Excitation in Gallates. <i>Materials Research Society Symposia Proceedings</i> , <b>2001</b> , 667, 1  Computation vs knowledge in materials innovation. <b>2001</b> , 4, 209-215  Physics and control of valence states in ZnO by codoping method. <b>2001</b> , 302-303, 155-162	3.3	97 2 4
476 475 474 473 472	Codoping method for the fabrication of low-resistivity wide band-gap semiconductors in p-type GaN, p-type AlN and n-type diamond: prediction versus experiment. <b>2001</b> , 13, 8901-8914  Electronic Structures and Nature of Host Excitation in Gallates. <i>Materials Research Society Symposia Proceedings</i> , <b>2001</b> , 667, 1  Computation vs knowledge in materials innovation. <b>2001</b> , 4, 209-215  Physics and control of valence states in ZnO by codoping method. <b>2001</b> , 302-303, 155-162  Control of valence states for ZnS by triple-codoping method. <b>2001</b> , 308-310, 916-919	3.3	97 2 4 146

468	A New Cubane-Type Ru4(CO)12(μ́3-Se)4 Tetramer Tailored for Water Photooxidation Catalysis. <b>2001</b> , 2001, 2489-2495		4
467	New valence control and spin control method in GaN and AlN by codoping and transition atom doping. <b>2001</b> , 231, 428-436		37
466	Electronic band structure of single-crystal and single-layer WS2: Influence of interlayer van der Waals interactions. <i>Physical Review B</i> , <b>2001</b> , 64,	3.3	151
465	Theoretical study on the phase stability, site preference, and lattice parameters for Gd(Fe, T)12. <b>2001</b> , 13, 2727-2736		64
464	Chapter 3 Magneto-optical kerr spectra. <b>2001</b> , 229-422		35
463	Magnetic, magneto-optical, and structural properties of URhAl from first-principles calculations. <i>Physical Review B</i> , <b>2001</b> , 63,	3.3	153
462	Electronic structure of CeNi2Ge2 investigated by angle-resolved photoemission and density-functional calculations. <i>Physical Review B</i> , <b>2001</b> , 64,	3.3	28
461	Experimental study of physical properties in the complex magnetic phase diagram of Ce(Rh1\( \text{Rhx}\) Rux)3B2. <i>Physical Review B</i> , <b>2001</b> , 64,	3.3	6
460	Magic behavior and bonding nature in hydrogenated aluminum clusters. <i>Physical Review B</i> , <b>2001</b> , 65,	3.3	79
459	Current-determined orbital magnetization in a metallic magnet. <i>Physical Review B</i> , <b>2001</b> , 63,	3.3	4
458	Correlation induced paramagnetic ground state in FeAl. <b>2001</b> , 87, 196401		90
457	Quantum electronic stability and spectroscopy of ultrathin Pb films on Si(111)7\(\bar{u}\). <i>Physical Review B</i> , <b>2002</b> , 66,	3.3	77
456	Electronic structure of Cs2KSb and K2CsSb. <i>Physical Review B</i> , <b>2002</b> , 66,	3.3	21
455	Quantitative theory of Invar-like anomalies in DyCo2 and HoCo2. <i>Physical Review B</i> , <b>2002</b> , 66,	3.3	12
454	Local symmetry breaking in paramagnetic insulating (Al,V)2O3. Physical Review B, 2002, 66,	3.3	8
453	SITE PREFERENCE AND VIBRATIONAL PROPERTIES OF Ni3Al WITH TERNARY ADDITIONS Pd AND Ag. <b>2002</b> , 16, 727-737		2
452	PHASE STABILITY OF ALKALI METALS UNDER PRESSURE: PERTURBATIVE AND NON-PERTURBATIVE TREATMENTS. <b>2002</b> , 16, 4847-4864		3
451	First-principle investigation of barrier height fluctuations in metal/oxide heterojunctions in relation with large tunnel current fluctuations. <b>2002</b> , 59, 742-748		3

450	The metal-insulator transition of NbO 2 : An embedded Peierls instability. <b>2002</b> , 58, 851-856	78
449	Exchange interactions and Curie temperature in (Ga,Mn)As. <i>Physical Review B</i> , <b>2002</b> , 66, 3.3	91
448	Magnetism of URhSi and URhGe: a density functional study. <b>2002</b> , 337, 48-52	18
447	Chemical bonding and magnetic trends within the ironflitrogen system. <b>2002</b> , 345, 72-76	27
446	Codoping for the fabrication of p-type ZnO. <b>2002</b> , 420-421, 100-106	142
445	Theoretical study of the relation between interfacial imperfection and transport properties in magnetic tunnel junctions. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2002</b> , 240, 114-116	5
444	Materials Design for p-Type ZnS with Blue Ag Emission by Triple-Codoping Method. 2002, 229, 371-375	18
443	Codoping Method for Solutions of Doping Problems in Wide-Band-Gap Semiconductors. <b>2002</b> , 193, 423-433	44
442	Effets chimiques et magnEovolumiques compEitifs dans les nitrures dEnsertion. <b>2002</b> , 5, 539-546	6
441	Calculated de Haas-van Alphen data and plasma frequencies of MgB2 and TaB2. <b>2002</b> , 121, 99-102	11
440	Ab initio study of the Fe intra- and inter-layer magnetic order in Fe/Ir(001) superlattices. 2003, 37, 311-320	3
439	Oscillatory interlayer magnetic coupling and induced magnetism in Fe/Nb multilayers. 2003, 26, 143-146	1
438	Ab initio study of ferromagnetic La0[5Ba0[5CoO3. <b>2003</b> , 115, 439-446	1
437	A model study for the breaking of N2 from CNx within DFT. <b>2003</b> , 5, 701-703	23
436	Chemical pressure and hydrogen insertion effects in CeNiln. <b>2003</b> , 5, 1385-1393	16
435	Atomistic modeling of RuAl and (RuNi)Al alloys. <b>2003</b> , 48, 695-700	25
434	Octahedral tilting in ACu3Ru4O12 (A=Na, Ca, Sr, La, Nd). <b>2003</b> , 370, 719-724	21
433	Structure and electronic properties of new model dinitride systems: a density-functional study of CN2, SiN2, and GeN2. <b>2003</b> , 373, 636-641	40

432	Lattice vibration of Ce1⊠ScxFe4Al8. <b>2003</b> , 64, 433-441		2
431	Site preference and vibrational properties of ScFexAl12\(\mathbb{B}\). Journal of Magnetism and Magnetic Materials, <b>2003</b> , 256, 381-389	2.8	12
430	Tight-binding parameters from the full-potential linear muffin-tin orbital method: A feasibility study on NiAl. <b>2003</b> , 236, 97-111		1
429	Instability of the rhodium magnetic moment as the origin of the metamagnetic phase transition in <b>B</b> eRh. <i>Physical Review B</i> , <b>2003</b> , 67,	3.3	78
428	Ab initio investigations in magnetic oxides. <b>2003</b> , 31, 239-299		56
427	Investigation of the Young's modulus of TiB needles in situ produced in titanium matrix composite. <b>2003</b> , 340, 80-87		66
426	Ab-initio calculation of enthalpies of formation of intermetallic compounds and enthalpies of mixing of solid solutions. <b>2003</b> , 11, 1095-1102		38
425	Site preference and vibrational properties of ScCuxAl12⊠. <b>2003</b> , 349, 41-48		9
424	Atomistic simulation of the lattice constants and lattice vibrations in RT4Al8 (R=Nd, Sm; T=Cr, Mn, Cu, Fe). <b>2003</b> , 352, 26-33		13
423	Ab-initio calculation of the elastic constants and thermal expansion coefficients of Laves phases. <b>2003</b> , 11, 23-32		357
423		3.3	357 66
	2003, 11, 23-32  Electronic structure, exchange interactions, and Curie temperature in diluted III-V magnetic	3-3	
422	Electronic structure, exchange interactions, and Curie temperature in diluted III-V magnetic semiconductors: (GaCr)As, (GaMn)As, (GaFe)As. <i>Physical Review B</i> , <b>2003</b> , 67,		66
422 421	Electronic structure, exchange interactions, and Curie temperature in diluted III-V magnetic semiconductors: (GaCr)As, (GaMn)As, (GaFe)As. <i>Physical Review B</i> , <b>2003</b> , 67,  Curie temperatures of zinc-blende half-metallic ferromagnets. <i>Physical Review B</i> , <b>2003</b> , 67,  Understanding the complex metallic element Mn. I. Crystalline and noncollinear magnetic structure	3.3	103
422 421 420	Electronic structure, exchange interactions, and Curie temperature in diluted III-V magnetic semiconductors: (GaCr)As, (GaMn)As, (GaFe)As. <i>Physical Review B</i> , <b>2003</b> , 67,  Curie temperatures of zinc-blende half-metallic ferromagnets. <i>Physical Review B</i> , <b>2003</b> , 67,  Understanding the complex metallic element Mn. I. Crystalline and noncollinear magnetic structure of EMn. <i>Physical Review B</i> , <b>2003</b> , 68,	3.3	66 103 205
422 421 420 419	Electronic structure, exchange interactions, and Curie temperature in diluted III-V magnetic semiconductors: (GaCr)As, (GaMn)As, (GaFe)As. <i>Physical Review B</i> , <b>2003</b> , 67,  Curie temperatures of zinc-blende half-metallic ferromagnets. <i>Physical Review B</i> , <b>2003</b> , 67,  Understanding the complex metallic element Mn. I. Crystalline and noncollinear magnetic structure of $\bigoplus$ Mn. <i>Physical Review B</i> , <b>2003</b> , 68,  From VO 2 to V 2 O 3: The metal-insulator transition of the Magnli phase V 6 O 11. <b>2003</b> , 61, 361-367	3-3	66 103 205 26
422 421 420 419 418	Electronic structure, exchange interactions, and Curie temperature in diluted III-V magnetic semiconductors: (GaCr)As, (GaMn)As, (GaFe)As. <i>Physical Review B</i> , <b>2003</b> , 67,  Curie temperatures of zinc-blende half-metallic ferromagnets. <i>Physical Review B</i> , <b>2003</b> , 67,  Understanding the complex metallic element Mn. I. Crystalline and noncollinear magnetic structure of BMn. <i>Physical Review B</i> , <b>2003</b> , 68,  From VO 2 to V 2 O 3: The metal-insulator transition of the Magnli phase V 6 O 11. <b>2003</b> , 61, 361-367  Orbital state and magnetic properties of LiV2O4. <i>Physical Review B</i> , <b>2003</b> , 67,  Efficient self-consistent calculations of multiband superconductivity in UPd2Al3. <i>Physical Review B</i> ,	3·3 3·3 3·3	66 103 205 26 35

414 Electron Structure of Solids. 2003,

413	Magnetism of cubic Mntaks compounds: anab initiostudy. <b>2004</b> , 16, 5869-5882		2
412	A first principle investigation of the polarized evanescent d states in Co/SrTiO3magnetic junctions. <b>2004</b> , 16, 1603-1612		1
411	Quasi-ab initiostudy on the structure and Curie temperature for Nd2Co17´xVxand (Nd1´xErx)2Co15.5V1.5. <b>2004</b> , 12, 871-880		2
410	Electronic structure and magnetic moment formation in Mnta As alloys. 2004, 16, S5661-S5667		
409	Magnetic properties of FeNi invar calculated in the dynamic non-local approximation of the spin fluctuation theory. <b>2004</b> , 16, 361-371		8
408	Full potential linearized augmented plane wave investigations of structural and electronic properties of pyrochlore systems. <b>2004</b> , 96, 6482-6487		31
407	Spin fluctuations in ferromagnetic ZrZn2. <i>Physical Review B</i> , <b>2004</b> , 70,	3.3	7
406	Electronic structure of paramagnetic V2O3: Strongly correlated metallic and Mott insulating phase. <i>Physical Review B</i> , <b>2004</b> , 70,	3.3	98
405	Ab initio approach of the hydrogen insertion effect on the magnetic properties of YFe2. <i>Physical Review B</i> , <b>2004</b> , 70,	3.3	39
404	Energy functional dependence of exchange coupling and magnetic properties of FeNb multilayers. <i>Physical Review B</i> , <b>2004</b> , 70,	3.3	9
403	3. Methods for Band Structure Calculations in Solids. <i>Lecture Notes in Physics</i> , <b>2004</b> , 23-54	0.8	2
402	Intrinsic Valence Band Study of Molecular-Beam-Epitaxy-Grown GaAs and GaN by High-Resolution Hard X-ray Photoemission Spectroscopy. <b>2004</b> , 43, L1029-L1031		31
401	First principles search of hard materials within the Si?C?N ternary system. 2004, 6, 315-323		16
400	Approach of charge disproportionation in the perovskite oxide TlNiO3 from ab initio electronic structures. <b>2004</b> , 6, 777-782		2
399	Interplay of Electronic Structure and Bulk Properties in 2D and 3D Ternary Carbonitrides from First Principles. <b>2004</b> , 630, 2587-2598		6
398	Theoretical study on the structure for R2Co17 (R=Y, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er) and R2Co17T (T=Be, C). <b>2004</b> , 65, 1307-1315		9
397	Extended moment formation and magnetic ordering in the trigonal chain compound Ca3Co2O6. <b>2004</b> , 385, 249-254		39

396	Charge order, orbital order, and electron localization in the Magnli phase Ti4O7. 2004, 390, 151-156		37
395	Ultrafast demagnetization in Ni: theory of magneto-optics for non-equilibrium electron distributions. <b>2004</b> , 16, 5519-5530		73
394	First-principles calculation of the intersublattice exchange interactions and Curie temperatures of the full Heusler alloys Ni2MnX (X=Ga,In,Sn,Sb). <i>Physical Review B</i> , <b>2004</b> , 70,	.3	229
393	Effect of H insertion on the magnetic, electronic, and structural properties of CeCoSi. <i>Physical Review B</i> , <b>2004</b> , 70,	.3	49
392	Ferromagnetism and temperature-dependent electronic structure of hcp gadolinium. <i>Physical Review B</i> , <b>2004</b> , 69,	.3	40
391	Calculated electronic properties of the mixed perovskite oxides: CaCu3T4O12 (T=Ti, Cr, Mn, Ru) within the DFT. <b>2004</b> , 58, 746-751		15
390	Magnetic exchange coupling and Curie temperature of . <i>Journal of Magnetism and Magnetic Materials</i> , <b>2005</b> , 290-291, 385-387	.8	7
389	A theoretical investigation of 4f- <b>d</b> d transition of trivalent rare earth ions in fluorides and complex oxides. <b>2005</b> , 114, 255-266		29
388	Structural imitation and lattice vibration of R2Co17⊠Mnx (R = Dy, Ho). <b>2005</b> , 335, 464-470		12
387	Atomistic simulation for the phase stability, site preference and thermal expansion of YFe12NTx (T=Ti, V, Cr, Mn, Zr, Nb, Mo, W). <b>2005</b> , 134, 771-776		25
386	Atomistic study on the structure and thermodynamic properties of Cr7C3, Mn7C3, Fe7C3. 2005, 53, 2727-	273	<b>2</b> 66
385	Ab initio investigation of the magnetic states of Ca2MnO4 and Ca2MnO3.5. <b>2005</b> , 310, 231-238		9
384	Pressure dependence of magnetic properties of CrO2 from theory. <b>2005</b> , 407, 516-521		14
383	Crystal Structure, Electronic Structure, and Luminescence of Cs2KYF6:Pr3+. <b>2005</b> , 631, 3046-3052		19
382	Atomistic study of structural simulation and Curie temperature of R2Fe17 $lambda$ Tx (R = Tb, Ho, Er; T = Ti, V, Cr, Mn). <b>2005</b> , 242, 1573-1580		2
381	Stability of ferromagnetism in the half-metallic pnictides and similar compounds: a first-principles study. <b>2005</b> , 17, 3915-30		57
380	Structural stability and site preference of Pr(Fe,M)12and Pr(Fe,M)12Nx(M= Ti, V, Cr, Mo). <b>2005</b> , 13, 851-86	50	3
379	Covalent bonding and hybridization effects in the corundum-type transition-metal oxides V $2$ O $3$ and Ti $2$ O $3$ . <b>2005</b> , 70, 782-788		37

378 Atomistic simulation on site preference and lattice vibrations of NdMn8T4(T = Fe, Co, Ni). **2005**, 38, 1199-1204 3

377	Pressure dependence of the Curie temperature in Ni2MnSn Heusler alloy: A first-principles study. <i>Physical Review B</i> , <b>2005</b> , 71,	3.3	120
376	Above-room-temperature ferromagnetism in half-metallic Heusler compounds NiCrP, NiCrSe, NiCrTe, and NiVAs: A first-principles study. <b>2005</b> , 98, 063523		42
375	Electronic structure of the antiferromagnetic semiconductor MnSb2S4. <i>Physical Review B</i> , <b>2005</b> , 71,	3.3	18
374	Importance of thermal disorder on the properties of alloys: Origin of paramagnetism and structural anomalies in bcc-based Fe1⊠Alx. <i>Physical Review B</i> , <b>2005</b> , 71,	3.3	38
373	Atomistic simulation on phase stability and site preference ofR2(Co, Mn)17(R= Nd, Sm, Gd). <b>2005</b> , 13, 239-247		12
372	First-principles study of exchange interactions and Curie temperatures of half-metallic ferrimagnetic full Heusler alloys Mn2V Z ( $Z = Al$ , Ge). <b>2005</b> , 17, 995-1001		90
371	Ab initio investigation of the nitrofluoride SiNF. <i>Physical Review B</i> , <b>2005</b> , 72,	3.3	6
370	Exchange interactions and temperature dependence of magnetization in half-metallic Heusler alloys. <i>Physical Review B</i> , <b>2005</b> , 72,	3.3	222
369	Electronic structure of Li-inserted V6O13 battery cathodes: Rigid band behavior and effects of hybridization. <b>2005</b> , 86, 064101		29
368	First principles study of the stability of SiNF. <b>2005</b> , 34, 22-34		3
367	Magnetic behavior of Fe sites in FeMoAl alloys: The role of the first neighborhood. <b>2005</b> , 29, 222-229		7
366	chapter 4 Magnetic and Electrical Properties of Practical Antiferromagnetic Mn Alloys. <b>2006</b> , 16, 209-40	)1	7
365	Ab initioestimates of the Curie temperature for magnetic compounds. <b>2006</b> , 18, 9795-9807		47
364	Exchange interactions and NBI temperature of a Fe monolayer on W(001): A first-principles study. <i>Physical Review B</i> , <b>2006</b> , 73,	3.3	15
363	A model study for the breaking of cyanogen out of CNx within DFT. <b>2006</b> , 15, 1609-1613		8
362	Electronic Structure Calculations. 2006,		1
361	Unusual sequence of phase transitions in MnAs: First-principles study. <i>Physical Review B</i> , <b>2006</b> , 74,	3.3	12

360	Half-Metallicity and Slater-Pauling Behavior in the Ferromagnetic Heusler Alloys. <i>Lecture Notes in Physics</i> , <b>2006</b> , 1-39	0.8	11
359	Hydrogen in Metals. 2006,		
358	Ferromagnetism in tetrahedrally coordinated compounds of I/II-V elements: Ab initio calculations. <i>Physical Review B</i> , <b>2006</b> , 73,	3.3	141
357	Phase stability and site preference of the disordered TbCu7-type compound PrCo7\(\text{QTx}\) (T=Ti, Zr, Hf, Cu). <b>2006</b> , 420, 1-8		8
356	Investigation of crystal structure and associated electronic structure of Sr6BP5O20. <b>2006</b> , 179, 968-973		22
355	Magnetic ground state of UCu2X2 (X=Si, Ge) from first principles. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2006</b> , 305, 264-268	2.8	6
354	Influence of Ce-H bonding on the physical properties of the hydrides CeCoSiH(1.0) and CeCoGeH(1.0). <b>2006</b> , 18, 6045-56		19
353	Spin-Polarized Electronic Structure. <b>2006</b> , 13-39		1
352	First-principles investigation of magnetism of U films and U(001)(1)/Fe(110)(3) multilayers. <b>2006</b> , 18, 4177-88		5
351	Exchange interactions in ZnMeO (Me=Mn,Fe,Co,Ni): Calculations using the frozen-magnon technique. <i>Physical Review B</i> , <b>2006</b> , 73,	3.3	33
350	Electron localization in metallic quantum wells: Pb versus In on Si(111). Physical Review B, 2006, 73,	3.3	53
349	Orbital ordering and spin-ladder formation in La2RuO5. <b>2006</b> , 96, 256401		24
348	poly-methyltrioxorhenium {(CH3)0.92ReO3}[]A conducting two-dimensional organometallic oxide. <i>Physical Review B</i> , <b>2006</b> , 73,	3.3	3
347	Half-metallic sp-electron ferromagnets in rocksalt structure: The case of SrC and BaC. <b>2007</b> , 91, 082512		81
346	Electronic and magnetic properties and chemical bonding of CeMSn (M=Rh,Ru) from first principles. <i>Physical Review B</i> , <b>2007</b> , 76,	3.3	38
345	First-principles study of the electronic and magnetic structures of the tetragonal and orthorhombic phases of Ca3Mn2O7. <i>Physical Review B</i> , <b>2007</b> , 76,	3.3	20
344	Characterization and electronic structure calculations of the antiferromagnetic insulator Ca3FeRhO6. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	4
343	Structural stability and magnetism of FeN from first principles. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	41

## (2007-2007)

342	Localization of oxygen donor states in gallium nitride from first-principles calculations. <i>Physical Review B</i> , <b>2007</b> , 76,	3.3	23
341	Mn-stabilized zirconia: from imitation diamonds to a new potential high-Tc ferromagnetic spintronics material. <b>2007</b> , 98, 016101		84
340	Ab initio analysis of magnetovolume versus chemical effects in CeRuSi and its hydride. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	15
339	An Approach for a Broad Search of New Compound Using the First Principles Calculation; AB Type Binary and Quaternary Intermetallic-Alloy. <b>2007</b> , 71, 860-868		
338	Structure, ordering, and bonding of half antiperovskites: PbNi3/2S and BiPd3/2S. 2007, 35, 309-327		41
337	Possible spin-Peierls transition in La2RuO5. <b>2007</b> , 35, 433-438		10
336	Ab-initio calculation of electronic structure and electric field gradients in HfAl2 and ZrAl2 Laves phases. <b>2007</b> , 41, 164-167		9
335	Ab initio studies of the electronic structure of the quaternary system LiBC4N4. <b>2007</b> , 427, 61-66		4
334	Pressure-induced delocalization in intermetallic system UMn2Ge2. 2007, 436, 34-37		4
333	Energetic evaluation of possible stacking structures of Li-intercalation in graphite using a first-principle pseudopotential calculation. <b>2007</b> , 439, 258-267		52
332	Heisenberg Hamiltonian description of multiple-sublattice itinerant-electron systems: General considerations and applications to NiMnSb and MnAs. <i>Physical Review B</i> , <b>2007</b> , 76,	3.3	41
331	Energy dependence of exact muffin-tin-orbital structure constants. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	14
330	Understanding the trend in the Curie temperatures of Co2-based Heusler compounds: Ab initio calculations. <i>Physical Review B</i> , <b>2007</b> , 76,	3.3	231
329	Experimental electron density of the complex carbides Sc3[Fe(C2)(2)] and Sc3[Co(C2)(2)]. <b>2007</b> , 129, 9356-65		46
328	Ab initio design of half-metallic fully compensated ferrimagnets: The case of Cr2MnZ (Z=P, As, Sb, and Bi). <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	134
327	Half-metallic ferromagnetism in zinc-blende CaC, SrC, and BaC from first principles. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	253
326	Calculated magneto-optical Kerr spectra of the half-Heusler compounds AuMnX (X = In, Sn, Sb). <b>2007</b> , 19, 315216		10
325	Cobalt Centered Trigonal RE6 Prisms and Mg4 Clusters as Basic Structural Units in RE4CoMg (RE = Y, La, Pr, Nd, Sm, Gd⊞m). <b>2007</b> , 633, 151-157		33

324	Ab initio investigation of the electronic structures of ternary germanides CeRhGe and CeIrGe. <b>2007</b> , 9, 274-278		21
323	Orbital ordering in the two-dimensional ferromagnetic semiconductor. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2007</b> , 312, L11-L15	2.8	2
322	Ab initio investigation of the electronic structure and the magnetic trends within equiatomic FeN. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2007</b> , 312, 298-304	2.8	11
321	Modification of the equation of state upon structural transition from two-dimensional branching of Ti2 dimers to a three-dimensional Ti13 cluster. <i>Physics of the Solid State</i> , <b>2007</b> , 49, 2210-2215	0.8	3
320	Atomistic Modeling of Multicomponent Systems. <b>2007</b> , 28, 23-37		О
319	Predicting metallic conductivity in oxides from simple chemical criteria. 2007, 68, 331-336		4
318	Molecular and all-solid DFT studies of the magnetic and chemical bonding properties within $KM[Cr(CN)6]$ (M = V, Ni) complexes. <b>2008</b> , 352, 85-91		5
317	Hyperfine magnetic field at Ta impurities in nickel: Perturbed angular correlation and first principle calculation study. <b>2008</b> , 145, 465-468		3
316	Ab initio investigation of perovskite and post-perovskite CaPtO3. 2008, 352, 92-96		6
315	Interplay of negative pressure and hydrogen chemical effects in CeRhSn from first principles. <b>2008</b> , 65, 491-498		5
314	Structure and properties of RERhZn (RE = La, Ce, Pr, Nd). 2008, 10, 1895-1904		18
313	Role of conduction electrons in mediating exchange interactions in Mn-based Heusler alloys. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	167
312	Structural, thermal, and electrical properties of CrSi2. <b>2008</b> , 103, 113516		66
311	Electronic structure calculations for inhomogeneous systems: Interfaces, surfaces, and nanocontacts. <i>Annalen Der Physik</i> , <b>2008</b> , 17, 525	2.6	
310	Long-range magnetic order and spin-lattice coupling in delafossite CuFeO2. <i>Physical Review B</i> , <b>2008</b> , 78,	3.3	29
309	Magnetic ordering in trigonal chain compounds. <b>2008</b> , 36, 156-161		3
308	Hydrogen insertion effects on the magnetic properties and chemical bonding within C14 Laves phases. <b>2008</b> , 36, 192-212		6
307	Thermal magnetic properties of the Ni sublattice in half-metallic NiMnSb: A theoretical study based on first-principles calculations. <i>Physical Review B</i> , <b>2008</b> , 78,	3.3	22

## (2009-2008)

306	Stability and magnetic properties of Mn-substituted ScN semiconductor from first principles. <b>2008</b> , 43, 392-398		12
305	A first-principle study of the site preference of Cd impurity in HfAg and ZrAg compounds. <b>2008</b> , 43, 867-871		2
304	Magnetic and electronic properties of double perovskites and estimation of their Curie temperatures by ab initio calculations. <i>Physical Review B</i> , <b>2008</b> , 78,	,	66
303	On the Metallic Conductivity of the Delafossites PdCoO2 and PtCoO2. <b>2008</b> , 20, 2370-2373		59
302	First principles study of the electronic and magnetic structures of U2Ni2SnH2. <b>2008</b> , 10, 083013		4
301	Embedded-cluster self-consistent partial-wave method: Extending the spatial scale of electronic structure calculations. <i>Physical Review B</i> , <b>2008</b> , 77,	;	1
300	Electronic structure of transition-metal impurities in semiconductors: Cu in GaP. <i>Physical Review B</i> , <b>2008</b> , 78,	i	9
299	Ab initio study of hyperfine interaction parameters in C14 Hf and Zr Laves-phase compounds.  Physical Review B, <b>2009</b> , 79,		6
298	Challenge of magnetism in strongly correlated open-shell 2p systems. <b>2009</b> , 102, 016401		39
297	Electronic structure and thermoelectric properties of CuRh1\(\mathbb{M}\)gxO2. <i>Physical Review B</i> , <b>2009</b> , 80, 3.3		44
296	Influence of pressure on the magnetic ordering of CeNiSnH and CeNiSnH(1.8) hydrides. <b>2009</b> , 21, 305601		4
295	Physical origin of the incommensurate spin spiral structure in Mn3Si. <b>2009</b> , 105, 07E506		10
294	Searching for Si-based spintronics by first principles calculations. <b>2009</b> , 11, 125009		13
293	First-principle study of hydrogen stability within TiCo3. <b>2009</b> , 11, 894-899		4
292	Investigation of changes in crystal and electronic structures by hydrogen within LaNi5 from first-principles. <b>2009</b> , 11, 1098-1106		15
291	Structure, chemical bonding, and 45Sc solid state NMR of Sc2RuSi2. <b>2009</b> , 11, 1239-1245		6
<b>2</b> 90	Electronic structure and chemical bonding properties of UO2F2 from first principles. <b>2009</b> , 11, 1380-1385		4
289	X-ray/neutron diffraction studies and ab initio electronic structure of CeMgNi4 and its hydride. <b>2009</b> , 11, 1971-1978		29

288	First principles studies of SnTiO3 perovskite as potential environmentally benign ferroelectric material. <b>2009</b> , 355, 43-49	69
287	Thermodynamic characterization of NiAl. <b>2009</b> , 41, 610-616	3
286	New Ternary Silicide LiRh2Si2 latructure and Bonding Peculiarities. 2009, 635, 1894-1903	13
285	Hydrogen and carbon interaction in a FeNi alloy with a vacancy. <b>2009</b> , 246, 1275-1285	3
284	On the strong impact of doping in the triangular antiferromagnet CuCrO2. <b>2009</b> , 149, 962-967	66
283	First-principles calculations of optical and magneto-optical properties of Ga1-xMnxAs and MnAs. <b>2009</b> , 404, 3782-3788	8
282	Electronic band structure of from first principles. <b>2009</b> , 182, 2678-2684	9
281	First principles studies of the electronic and magnetic structures of [Fe(pz)2]x complex. <b>2009</b> , 359, 14-20	2
280	Ab initio molecular simulations with numeric atom-centered orbitals. <b>2009</b> , 180, 2175-2196	1637
279	First principles studies of ZrNi and ZrNiH3. <b>2009</b> , 473, 61-65	23
279 278	First principles studies of ZrNi and ZrNiH3. 2009, 473, 61-65  Electronic structure and lattice anisotropy of . 2009, 476, 213-217	3
278	Electronic structure and lattice anisotropy of . <b>2009</b> , 476, 213-217	3
278 277	Electronic structure and lattice anisotropy of . <b>2009</b> , 476, 213-217  Electric field gradients at Ta and Cd in Ti2Pd compound. <b>2009</b> , 477, 36-39  Experimental and ab initio study of the electric field gradients at Ta and Cd impurities in TiAl3. <b>2009</b>	3
278 277 276	Electronic structure and lattice anisotropy of . <b>2009</b> , 476, 213-217  Electric field gradients at Ta and Cd in Ti2Pd compound. <b>2009</b> , 477, 36-39  Experimental and ab initio study of the electric field gradients at Ta and Cd impurities in TiAl3. <b>2009</b> , 479, 56-59  Huge influence of hydrogenation on the magnetic properties and structures of the ternary silicide	3 1 3
278 277 276 275	Electric field gradients at Ta and Cd in Ti2Pd compound. 2009, 477, 36-39  Experimental and ab initio study of the electric field gradients at Ta and Cd impurities in TiAl3. 2009, 479, 56-59  Huge influence of hydrogenation on the magnetic properties and structures of the ternary silicide NdMnSi. 2009, 106, 033910	3 1 3
278 277 276 275 274	Electric field gradients at Ta and Cd in Ti2Pd compound. 2009, 477, 36-39  Experimental and ab initio study of the electric field gradients at Ta and Cd impurities in TiAl3. 2009, 479, 56-59  Huge influence of hydrogenation on the magnetic properties and structures of the ternary silicide NdMnSi. 2009, 106, 033910  Intermetallic hydrides: A review with ab initio aspects. 2010, 38, 1-37  YNi and its hydrides: Phase stabilities, electronic structures and chemical bonding properties from	3 1 3 14 71

# (2010-2010)

270	Atomistic simulation for disordered TbCu7-type compounds SmCo7 and Sm(Co,T)7 (T=Ti, Ga, Si, Cu, Hf, Zr). <b>2010</b> , 12, 33-38		18
269	DFT study of hydrogen instability and magnetovolume effects in CeNi. <b>2010</b> , 12, 59-64		9
268	DFT study of electronic and magnetic structure of perovskite and post-perovskite CaRhO3. <b>2010</b> , 12, 373-378		15
267	The plumbide CeZnPb lbtructure, magnetism, and chemical bonding. 2010, 12, 929-937		11
266	Potential existence of anti-postperovskite iron nitride Fe4N. <b>2010</b> , 12, 1131-1135		2
265	Calculated structural properties of TbCu7-type disordered intermetallic compounds NdCo7 and Nd1 $\square$ YxCo6.8Zr0.2 (x´= 0, 0.2, 0.4, 0.6). <b>2010</b> , 12, 1711-1719		1
264	AMoO4 (A´=´Mg, Ni) molybdates: Phase stabilities, electronic structures and chemical bonding properties from first principles. <b>2010</b> , 12, 1779-1785		31
263	Site preference and vibrational properties of R3T4+xAl12☑ (R=Y, Ce, Gd, U, Th; T=Fe, Ru). <b>2010</b> , 183, 504-509		3
262	Potential existence of post-perovskite nitrides; DFT studies of ThTaN3. <b>2010</b> , 183, 994-999		11
261	Does a Heisenberg Hamiltonian describe magnetic interactions in a MnSi film properly?. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2010</b> , 322, 1082-1084	2.8	2
260	Exchange mechanism of half-metallic ferromagnetism of TiO2 doped with double impurities: A first-principles ASW study. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2010</b> , 322, 454-458	2.8	15
259	DFT study of magneto-volume effects in iron and cobalt nitrides. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2010</b> , 322, 658-660	2.8	24
258	Lattice anisotropy, electronic and chemical structures of uranyl carbonate, UO2CO3, from first principles. <b>2010</b> , 372, 46-50		6
257	Ternary Silicides Sc3TSi3 (T = Ru, Rh, Ir, Pt) Latructure, Chemical Bonding, and Solid State NMR´. <b>2010</b> , 636, 1839-1850		10
256	Complex Borides RERu4B4 (RE = Ce, Pr, Nd, Sm) [Bonding Peculiarities and Magnetic Properties'. <b>2010</b> , 636, 1236-1241		1
255	An atomistic simulation of the structural and vibrational properties of A4Fe3Al32(A= Th, U). <b>2010</b> , 18, 045002		11
254	Linear Muffin-Tin Orbital Method in the Atomic Sphere Approximation. 2010, 35-46		
253	Stable and variable features of the magnetic structure of fcc Fe/Cu(001) films. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	14

252	New Hydrides REScSiH and REScGeH (RE = La, Ce): Structure, Magnetism, and Chemical Bonding. <b>2010</b> , 22, 5013-5021		19
251	Hydrogenation inducing ferromagnetism in the ternary antiferromagnet NdCoSi. <b>2010</b> , 49, 4836-42		22
250	Electronic structure of solids with WIEN2k. <b>2010</b> , 108, 3147-3166		86
249	Composition-Dependent Basics of Smart Heusler Materials from First- Principles Calculations. <b>2011</b> , 684, 1-29		34
248	New Quaternary Hydride CeZnSnH1.5: Structure, Magnetism, and Chemical Bonding. <b>2011</b> , 23, 1096-110	4	9
247	Magnetic excitations and femtomagnetism of FeRh: A first-principles study. <i>Physical Review B</i> , <b>2011</b> , 83,	3.3	72
246	Structural-induced antiferromagnetism in Mn-based full Heusler alloys: The case of Ni2MnAl. <b>2011</b> , 98, 102514		45
245	Electronic properties of oxides: Chemical and theoretical approaches. <b>2011</b> , 39, 70-95		53
244	Stability of ferromagnetism against doping in half-metallic alloys. <b>2011</b> , 109, 113912		10
243	Ab initio investigations of the perovskite and K2NiF4 phases in the Csta⊞ system. <b>2011</b> , 13, 569-573		3
242	Ab initio study of the hydrogenation effects on the electronic, chemical, and magnetic structures of CeIrSb. <b>2011</b> , 13, 948-952		4
241	Crystal and electronic structure of LaPdSn and RE3Pd4Sn6 (RE´=´La, Ce). <b>2011</b> , 13, 1285-1290		5
240	Ab initio investigations of the Ca2IrO4-type structure as a post-K2NiF4ECase study of Na2OsO4. <b>2011</b> , 13, 1396-1400		8
239	First principles investigations of the hydrogenation effects on the electronic structure and the chemical bonding of CeIrAl. <b>2011</b> , 13, 1704-1708		5
238	First-principles study of electronic structure and magnetic properties of doped SnO2 (rutile) with single and double impurities. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2011</b> , 323, 2982-2986	2.8	17
237	Palladium site ordering and the occurrence of superconductivity in Bi2Pd3Se2⊠Sx. <b>2011</b> , 184, 797-804		10
236	Oxygen adsorption on Al (111) surface interstitial site calculated by density functional theory. <b>2011</b> , 43, 940-944		6
235	Electronic structure and equation of state of PdO2 from ab initio. <b>2011</b> , 508, 215-218		19

234	Variation of the magnetic properties of Ni2MnGa Heusler alloy upon tetragonalization: a first-principles study. <b>2011</b> , 44, 235001		21
233	High TC half-metallic fully-compensated ferrimagnetic Heusler compounds. <b>2011</b> , 99, 052509		104
232	Electron-phonon scattering dynamics in ferromagnetic metals and their influence on ultrafast demagnetization processes. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	65
231	Exchange interactions, spin waves, and Curie temperature in zincblende half-metallic sp-electron ferromagnets: the case of CaZ ( $Z = N, P, As, Sb$ ). <b>2011</b> , 23, 296001		17
230	A tight binding model for water. <b>2011</b> , 134, 044130		10
229	Ab initio investigation of the mechanical properties of copper. <b>2012</b> , 21, 096102		9
228	Berry curvature and the anomalous Hall effect in Heusler compounds. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	64
227	Introduction. Lecture Notes in Physics, 2012, 1-4	0.8	
226	Half-metallic antiferromagnetism in Cr2+xSe (0個1): A first-principles study. <i>Physical Review B</i> , <b>2012</b> , 86,	3.3	17
225	Ab-initio calculation of effective exchange interactions, spin waves, and Curie temperature in L21-and L12-type local moment ferromagnets. <b>2012</b> , 47, 7678-7685		11
224	Intermediate cerium valence intermetallics Ce4RuMg, Ce23Ru7Mg4, CeRu2Mg5, and Ce2Ru4Mg17: Electronic structures and chemical bonding from DFT. <b>2012</b> , 31, 88-93		11
223	Transition metal hydrido-complexes: Electronic structure and bonding properties. <b>2012</b> , 40, 31-40		7
222	Underpinning energetics of lithium bonding and stability in the LiPtBn system. 2012, 14, 1471-1475		4
221	First principles investigations of the electronic structure and chemical bonding of U3Si2C2 IA uranium silicidelarbide with the rare [SiC] unit. <b>2012</b> , 550, 88-93		5
220	Dimorphic LaPdSn and ErAgSn 🖟 first principles study. <b>2012</b> , 20, 33-38		5
219	Electronic structure and chemical bonding of Li4Pt3Si. <b>2012</b> , 542, 47-51		2
218	Robustness and stability of half-metallic ferromagnetism in alkaline-earth metal mononitrides against doping and deformation. <b>2012</b> , 111, 113918		7
217	Ab initio investigations of the electronic structure and lithium stability in Li2UN2 and LiUN2. <b>2012</b> , 143, 1341-1348		2

216	Ferromagnetism in Mo-doped TiO2 Rutile from Ab Initio Study. <b>2012</b> , 25, 503-507	13
215	Ab initio investigation of the electronic structure of CeRh2Sb2. <b>2012</b> , 537, 48-52	
214	Electronic structure and anisotropic chemical bonding in TiNF from ab initio study. <b>2012</b> , 185, 25-30	6
213	Electronic structure and chemical bonding of ⊞and EceIr2Si2 intermediate valence compounds. <b>2012</b> , 186, 81-86	5
212	Ab initio investigations of the electronic structure and chemical bonding of Li2ZrN2. <b>2012</b> , 190, 191-195	5
211	Electronic structure and chemical bonding of LiYSi. <b>2012</b> , 14, 375-380	6
<b>21</b> 0	7Li and 29Si solid state NMR and chemical bonding of La2Li2Si3. <b>2012</b> , 14, 367-374	8
209	Electronic structure and bonding of the hydrides Mg3TH7 (T´=´Mn, Re) from first principles. <b>2012</b> , 14, 639-643	2
208	The predominance of the rutile phase of SnO2: First principles study. <b>2012</b> , 152, 349-353	4
207	Structure identification and site preference of Ta and Cd in TiPd alloys: A first-principle study. <b>2012</b> , 152, 1072-1075	7
206	Half-metallic antiferromagnetic behavior of double perovskite Sr2OsMoO6: First principle calculations. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2013</b> , 345, 195-200	21
205	Linear infinite cadmium chains in CaAu4Cd2 and other intermetallics with YbMo2Al4-type structure. <b>2013</b> , 144, 751-760	15
204	First principles study of the electronic and magnetic structures and bonding properties of UCoC2 ternary, characteristic of CL units. <b>2013</b> , 17, 128-133	1
203	Changes in electronic, magnetic and bonding properties from Zr2FeH5 to Zr3FeH7 addressed from ab initio. <b>2013</b> , 25, 55-62	1
202	The ternary germanides UMnGe and U2Mn3Ge. <b>2013</b> , 21, 73-80	3
201	Drastic changes of electronic, magnetic, mechanical and bonding properties in Zr2Co by hydrogenation. <b>2013</b> , 36, 25-30	7
200	Ab initio investigation of the crystal and electronic structures of 'the 'nitride fluoride ThNF. <b>2013</b> , 18, 123-126	4
199	Realization of spin gapless semiconductors: the Heusler compound Mn2CoAl. <b>2013</b> , 110, 100401	339

198	Change of the cerium valence with temperature latructure and chemical bonding of HT-CeRhGe. <b>2013</b> , 21, 6-10	16
197	Ab initio investigations of the electronic structures and chemical bonding in LiCo6P4 and Li2Co12P7. <b>2013</b> , 202, 227-233	4
196	Half-metallic behaviour in doped TiO2 (rutile) with double impurities: ab initio calculation. <b>2013</b> , 86, 1178-118	351
195	Drastic changes in electronic, magnetic, mechanical and bonding properties from Zr2CoH5 to Mg2CoH5. <b>2013</b> , 200, 209-214	5
194	ScPdZn and ScPtZn with YAlGe Type Structure © Group-Subgroup Relation and 45Sc Solid State NMR Spectroscopy. <b>2013</b> , 639, 246-253	6
193	Full-Potential Study of the Magneto-Optical Kerr Effect for AuMnSb and AuMnSn. <b>2013</b> , 750-752, 941-945	2
192	Atomistic simulation of the lattice constants and lattice vibrations in RCo2 and Nd1 $\bar{l}$ k R x Co2 (R = rare earth). <b>2013</b> , 1, 81-89	3
191	Photocatalytic and Antipathogenic Effects of TiO2/CuxO (1. <b>2013</b> , 57, 483-488	
190	Non-vanishing Berry phase in chiral insulators. <b>2013</b> , 104, 30001	5
189	Hf dopants in <b>M</b> i3Al alloy. <b>2013</b> , 114, 063712	3
188	AB INITIO MOLECULAR DYNAMICS SIMULATIONS ON LOCAL STRUCTURE AND ELECTRONIC PROPERTIES IN LIQUID MgxBi1-x ALLOYS. <b>2013</b> , 27, 1350011	1
187	Theory of Hyperfine Interactions in Metals. <b>2013</b> , 101, 11-77	3
186	Magnesium and Cadmium in Covalently-Bonded Lonsdaleite Networks: Synthesis, Structure, and Bonding of AETMg2 and SrTCd2 (AE = Ca, Sr; T = Pd, Ag, Pt, Au). <b>2013</b> , 639, 707-713	9
185	References. <b>2014</b> , 299-302	
184	Non-collinear antiferromagnets and the anomalous Hall effect. <b>2014</b> , 108, 67001	177
183	Comparison between theoretical and experimental results for energy states of two-dimensional electron gas in pseudomorphically strained InAs high-electron-mobility transistors. <b>2014</b> , 53, 04EF09	4
182	Drastic changes in the electronic and magnetic structures of hydrogenated U2Ti intermetallic from first principles. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2014</b> , 358-359, 70-75	4
181	Electronic and magnetic structures and bonding properties of Ce2T2X ( $T'='$ nd element; $X'='$ Mg, Cd, Pb or Sn) intermetallics from first principles. <b>2014</b> , 51, 18-23	8

180	Electronic structures and ferromagnetism of SnO2 (rutile) doped with double-impurities: First-principles calculations. <b>2014</b> , 115, 013910		6
179	Electronic structure and crystal phase stability of palladium hydrides. <b>2014</b> , 116, 173706		32
178	The Family of LiCo6P4 Type Compounds Drends in Electronic Structure and Chemical Bonding. <b>2014</b> , 640, 1641-1647		5
177	Half metallic antiferromagnetic behavior in doped TiO2 rutile with double impurities (Os, Mo) from ab initio calculations. <b>2014</b> , 570, 45-48		7
176	Electronic structure and peculiar bonding properties of NdNiMg5 from first principles. <b>2014</b> , 38, 1-6		5
175	Pressure induced metallization of fordite SnNb2O6 from first principles. <b>2014</b> , 84, 355-359		2
174	In silico CrNF, a half-metallic ferromagnetic nitridefluoride mimicking CrO2. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2014</b> , 368, 105-110	2.8	7
173	The U4Re7Si6 type ITrends in electronic structure and chemical bonding. <b>2014</b> , 27, 5-10		4
172	Drastic changes of electronic structure, bonding properties and crystal symmetry in Zr2Cu by hydrogenation, from ab initio. <b>2014</b> , 45, 5-10		3
171	A bridge for accelerating materials by design. <b>2015</b> , 1,		33
170	Ab initio investigation of light-induced relativistic spin-flip effects in magneto-optics. <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	22
169	Coherent view of crystal chemistry and ab initio analyses of Pb(II) and Bi(III) lone pair in square planar coordination. <b>2015</b> , 43, 82-97		- T
	planar coordination. 2013, 43, 62 31		15
168	LaMgX and CeMgX (X´=´Ga, In, Tl, Pd, Ag, Pt, Au) with ZrNiAl type structure [A systematic view on electronic structure and chemical bonding. <b>2015</b> , 43, 28-34		2
168 167	LaMgX and CeMgX (X´=´Ga, In, Tl, Pd, Ag, Pt, Au) with ZrNiAl type structure 🗗 systematic view on		
	LaMgX and CeMgX (X´=´Ga, In, Tl, Pd, Ag, Pt, Au) with ZrNiAl type structure [A systematic view on electronic structure and chemical bonding. <b>2015</b> , 43, 28-34		
167	LaMgX and CeMgX (X´=´Ga, In, Tl, Pd, Ag, Pt, Au) with ZrNiAl type structure [A systematic view on electronic structure and chemical bonding. <b>2015</b> , 43, 28-34  Rhodium-rich germanides RERh4Ge2 (RE = Y, Gd[lu): structure and bonding. <b>2015</b> , 146, 1375-1383		2
167 166	LaMgX and CeMgX (X'='Ga, In, Tl, Pd, Ag, Pt, Au) with ZrNiAl type structure IA systematic view on electronic structure and chemical bonding. 2015, 43, 28-34  Rhodium-rich germanides RERh4Ge2 (RE = Y, GdIIu): structure and bonding. 2015, 146, 1375-1383  Local structure study of Fe dopants in NiBeficit Ni3Al alloys. 2015, 651, 705-711  Chemical bonding in equiatomic cerium intermetallics IThe case of CeMgSn, CePdSn, and CeMgPb.		4

162	Crystal and chemical anisotropy effects in AE2ZnN2, (AE = Ca, Sr, Ba) from ab initio. 2015, 39, 10-14	3
161	Analysis of energy states of two-dimensional electron gas in pseudomorphically strained InSb high-electron-mobility transistors taking into account the nonparabolicity of the conduction band. <b>2016</b> , 55, 084301	1
160	Electronic and magnetic structures and bonding properties of Ce 2 CrN 3 and U 2 CrN 3 from first principles. <b>2016</b> , 9, 13-18	2
159	Drastic changes of electronic structure and crystal chemistry upon oxidation of SnII2TiO4E2 into SnIV2TiO6: An ab initio study. <b>2016</b> , 59, 25-31	1
158	Itinerant G-type antiferromagnetism in D03-type V3Z (Z=Al, Ga, In) compounds: A first-principles study. <i>Physical Review B</i> , <b>2016</b> , 94,	12
157	Electronic structure of FeAl alloy studied by resonant photoemission spectroscopy and Ab initio calculations. <b>2016</b> , 688, 187-194	14
156	Quaternary Germanides RE3TRh4Ge4 (RE = Ce, Pr, Nd; $T = Nb$ , Ta) $\Box$ A New Coloring Variant of the Aristotype AlB2. <b>2016</b> , 642, 979-986	4
155	A ZrNiAl related high-pressure modification of CeRuSn. <b>2016</b> , 45, 14216-29	5
154	Ternary silicides ScIr4Si2 and RERh4Si2 (RE = Sc, Y, Tb-Lu) and quaternary derivatives RERh4Si2\(\text{\text{BS}}\) Snx (RE = Y, Nd, Sm, Gd-Lu) \(\text{\text{\text{\text{\text{B}}}}\) Istructure, chemical bonding, and solid state NMR spectroscopy. <b>2016</b> , 231, 475-486	4
153	Analysis of energy states where electrons and holes coexist in pseudomorphically strained InAs high-electron-mobility transistors. <b>2016</b> , 55, 04EG08	
152	Tl(I) to Po(IV) 6s2 lone pairs in tetrahedral, triangular bipyramidal, square pyramidal, octahedral and hexahedral geometries: Crystal chemistry and ab initio visualizations and analyses. <b>2016</b> , 44, 35-58	8
151	Weyl points in the ferromagnetic Heusler compound Co 2 MnAl. <b>2016</b> , 114, 47005	69
150	The effect of fluorine doping on electronic structure and ferromagnetic stability of Os-doped TiO 2 rutile phase: First-principles calculations. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2016</b> , 401, 977-981	8
149	Dimorphic HT- and LT-TbTiGe: Electronic and magnetic structures and bonding properties from first principles. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2016</b> , 397, 275-280	
148	Electronic structure and chemical bonding in LaIrSi-type intermetallics. 2017, 72, 207-213	3
147	The nitridoborate nitrides Mg3[BN2]N and Ca3[BN2]N [electronic structure and chemical bonding. <b>2017</b> , 72, 433-439	
146	First-principles investigations of the electronic and magnetic structures and the bonding properties of uranium nitride fluoride (UNF). <b>2017</b> , 72, 725-730	1
145	Atomic structure governed diversity of exchange-driven spin helices in Fe nanoislands: Experiment and theory. <i>Physical Review B</i> , <b>2017</b> , 96,	1

144	Magneto-Optical Detection of the Spin Hall Effect in Pt and W Thin Films. 2017, 119, 087203		61
143	(CaO)nIrO2 (n = 1, 2, 4) family: Chemical scissors effects of CaO on structural characteristics correlated to physical properties. Ab initio study. <b>2017</b> , 255, 82-88		7
142	Insight into the Dzyaloshinskii-Moriya interaction through first-principles study of chiral magnetic structures. <i>Physical Review B</i> , <b>2017</b> , 96,	3.3	21
141	First principles studies of hydrogen insertion effects on magnetic properties, bonding and structure reordering of UZr 2. <b>2017</b> , 12, 19-24		1
140	Systematic First-Principles Study of Binary Metal Hydrides. <b>2017</b> , 19, 513-523		19
139	Weyl fermions in antiferromagnetic Mn 3 Sn and Mn 3 Ge. <b>2017</b> , 120, 47002		30
138	Ab Initio Methods. <b>2018</b> , 7-197		2
137	Antiferromagnetism and phase transitions in noncentrosymmetric UIrSi3. <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	8
136	Rare earth-rich compounds RE9TMg4 (RE = Y, Dy-Tm, Lu; T = Ru, Rh, Os, Ir) with an ordered Co2Al5-type structure. <b>2018</b> , 82, 70-77		8
135	High pressure in solid state chemistry: Combined experimental and modeling approaches for assessing and predicting properties. <b>2018</b> , 80, 178-195		1
134	The alkaline earth-palladium-germanides Sr3Pd4Ge4 and BaPdGe. 2018, 73, 243-250		2
133	Combined crystal chemistry and DFT studies of ThNCl and Th2N2X (X: chalcogen) behaving as pseudo-binaries. <b>2018</b> , 76, 1-7		
132	Magnetic field effect on the chiral magnetism of noncentrosymmetric UPtGe: Experiment and theory. <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	1
131	One-step hydrogen extraction and storage in plasma generated palladium nanoparticles. <b>2018</b> , 20, 1		3
130	Applications Perspectives of Nanodispersed Chalcogenides of Transition Metals in Photocatalysis. <b>2018</b> , 99-113		1
129	Correlations of Crystal and Electronic Structure via NMR and X-ray Photoelectron Spectroscopies in the RETMAl (RE = Sc, Y, La-Nd, Sm, Gd-Tm, Lu; TM = Ni, Pd, Pt) Series. <b>2019</b> , 58, 7010-7025		10
128	Magnetic phase transitions induced by pressure and magnetic field: The case of antiferromagnetic USb2. <i>Physical Review B</i> , <b>2019</b> , 99,	3.3	4
127	Coloring in the ZrBeSi-type structure. <b>2019</b> , 74, 307-318		4

#### (2020-2019)

ZrNiAl-type gallides with pronounced metal-metal bonding, and the dimorphism of ScPdGa. 2019, 126 2 74, 15-25 First principles investigations of Fe, Co, Ni in model honeycomb carbon networks. 2019, 87, 155-162 125 Rare-earth-doped TiO rutile as a promising ferromagnetic alloy for visible light absorption in solar 6 124 cells: first principle insights.. **2020**, 10, 35505-35515 Electron and phonon band structures of palladium and palladium hydride: A review. 2020, 60, 100285 123 Preface. 2020, xix-xxiii 122 Introduction. 2020, 1-14 121 Overview. 2020, 15-59 120 Theoretical Background. 2020, 60-80 119 118 Periodic Solids and Electron Bands. 2020, 81-108 Uniform Electron Gas and sp-Bonded Metals. 2020, 109-128 117 Density Functional Theory: Foundations. 2020, 129-144 116 The KohnBham Auxiliary System. 2020, 145-170 115 Functionals for Exchange and Correlation I. 2020, 171-187 114 Functionals for Exchange and Correlation II. 2020, 188-214 113 Electronic Structure of Atoms. 2020, 215-229 112 Pseudopotentials. **2020**, 230-258 111 Overview of Chapters 1218. 2020, 259-261 110 Plane Waves and Grids: Basics. 2020, 262-282 109

Plane Waves and Real-Space Methods: Full Calculations. 2020, 283-294 108 Localized Orbitals: Tight-Binding. 2020, 295-319 107 Localized Orbitals: Full Calculations. 2020, 320-331 106 Augmented Functions: APW, KKR, MTO. 2020, 332-364 105 Augmented Functions: Linear Methods. 2020, 365-385 104 Locality and Linear-Scaling O(N) Methods. 2020, 386-410 103 Quantum Molecular Dynamics (QMD). 2020, 411-426 102 Response Functions: Phonons and Magnons. 2020, 427-445 101 Excitation Spectra and Optical Properties. 2020, 446-464 100 Surfaces, Interfaces, and Lower-Dimensional Systems. 2020, 465-480 99 98 Wannier Functions. 2020, 481-498 Polarization, Localization, and Berry Phases. 2020, 499-516 97 96 Topology of the Electronic Structure of a Crystal: Introduction. 2020, 517-530 Two-Band Models: Berry Phase, Winding, and Topology. 2020, 531-546 95 Topological Insulators I: Two Dimensions. 2020, 547-568 94 Topological Insulators II: Three Dimensions. **2020**, 569-580 93 Functional Equations. 2020, 581-583 92 LSDA and GGA Functionals. 2020, 584-586 91

## (2020-2020)

90	Adiabatic Approximation. <b>2020</b> , 587-589		
89	Perturbation Theory, Response Functions, and Green Functions. 2020, 590-599		
88	Dielectric Functions and Optical Properties. <b>2020</b> , 600-606		
87	Coulomb Interactions in Extended Systems. <b>2020</b> , 607-619		
86	Stress from Electronic Structure. <b>2020</b> , 620-626		
85	Energy and Stress Densities. <b>2020</b> , 627-636		
84	Alternative Force Expressions. <b>2020</b> , 637-643		
83	Scattering and Phase Shifts. <b>2020</b> , 644-646		
82	Useful Relations and Formulas. <b>2020</b> , 647-650		
81	Numerical Methods. <b>2020</b> , 651-660		
80	Iterative Methods in Electronic Structure. <b>2020</b> , 661-676		
79	Two-Center Matrix Elements: Expressions for Arbitrary Angular Momentum l. <b>2020</b> , 677-685		
78	Dirac Equation and SpinDrbit Interaction. <b>2020</b> , 686-696		
77	Berry Phase, Curvature, and Chern Numbers. <b>2020</b> , 697-700		
76	Quantum Hall Effect and Edge Conductivity. <b>2020</b> , 701-703		
75	Index. <b>2020,</b> 756-762		
74	Complex interplay of magnetic interactions in 5f-electron systems: The case of U2Ni2Sn. <i>Physical Review B</i> , <b>2020</b> , 101,	3.3	3
73	Microscopic nature of drastic influence of hydrogen on the magnetic anisotropy of 5f-electron systems: The case of U2Ni2Sn. <i>Physical Review B</i> , <b>2020</b> , 101,	3.3	4

72	First-principles studies of the electronic and magnetic structures and bonding properties of boron subnitride B13N2. <b>2021</b> , 294, 121840		1
71	rhB12 as host of interstitial atoms: Review of a large family with illustrative study of B12{CN2} from first-principles. <b>2021</b> , 61, 100296		2
70	Ferromagnetic alloy for high-efficiency photovoltaic conversion in solar cells: first-principles insights when doping SnO rutile with coupled Eu-Gd <b>2021</b> , 11, 7096-7106		3
69	Interplay of spin magnetism, orbital magnetism, and atomic structure in layered van der Waals ferromagnet VI3. <i>Physical Review B</i> , <b>2021</b> , 103,	3.3	3
68	Quantum approximate methods for the atomistic modeling of multicomponent alloys. <b>2007</b> , 215-254		1
67	Advanced Ceramics and Nanocomposites of Half-metallic Ferromagnetic CrO2 for Magnetic, GMR and Optical Sensors. <b>2008</b> , 1-64		1
66	The Band Model for d- and f-Metals. NATO ASI Series Series B: Physics, 1984, 183-241		4
65	Electronic Structure of Hydrogen in Metals. NATO ASI Series Series B: Physics, 1984, 243-343		5
64	A First Principles Approach to the Band Theory of Random Metallic Alloys. <i>NATO ASI Series Series B: Physics</i> , <b>1984</b> , 463-579		10
63	Alloy Phase Diagrams From First Principles. NATO ASI Series Series B: Physics, 1984, 581-592		4
62	The Ideal Strength of Solids. 1983, 95-165		31
61	Introduction. <b>1997</b> , 1-36		3
60	Interpretation of the X-Ray Emission Spectra from FeAl, CoAl and NiAl. 1981, 631-634		1
59	Total Energy and Force Calculations with the LMTO Method. <b>1989</b> , 1-13		2
58	Current Ideas and Methods for Calculation of Ground State Properties of Solids. <b>1985</b> , 175-225		3
57	Electronic Structure of Metal Hydrides. <b>1981</b> , 215-242		7
56	Applications of Density Functional Theory to Atoms, Molecules, and Solids. <b>1983</b> , 189-308		28
55	Density Functional Approach to the Electronic Structure of Metal Surfaces and Metal-Adsorbate Systems. <b>1983</b> , 309-389		24

54	Hydrogen in Disordered Solids: Model and Calculations. NATO ASI Series Series B: Physics, 1986, 153-172	7	
53	Self-Consistent Band Structure and Fermi Surface for E(BEDT-TTF)213. <b>1990</b> , 208-211	1	
52	Electron Spectroscopy of Graphite Intercalation Compounds. <b>1992</b> , 53-104	5	
51	Electrons and Ions in Liquid and Amorphous Metals. <b>1984</b> , 211-230	2	
50	Electronic Structure Calculations for Rare Earth-Transition Metal Compounds. <b>1991</b> , 133-170	15	
49	Electronic Structure Methods. <b>1997</b> , 195-238	3	
48	Quantum Mechanical Calculations of Chemical Interactions on Transition Metal Surfaces. <b>1992</b> , 253-359	2	
47	Electronic structure determination. <b>1983</b> , 126-143	6	
46	ELECTRONIC STRUCTURE CALCULATION FOR THE METASTABLE Fe3B ALLOY. <b>1985</b> , 1031-1034	1	
45	Electronic Structure: Basic Theory and Practical Methods. <b>2020</b> ,	38	
45	Electronic Structure: Basic Theory and Practical Methods. 2020,  THEORY OF THE MAGNETO-OPTICAL PROPERTIES OF TRANSITION METALS AND RARE EARTH COMPOUNDS. Journal of the Magnetics Society of Japan, 1991, 15, S1_73-78	38	
	THEORY OF THE MAGNETO-OPTICAL PROPERTIES OF TRANSITION METALS AND RARE EARTH		
44	THEORY OF THE MAGNETO-OPTICAL PROPERTIES OF TRANSITION METALS AND RARE EARTH COMPOUNDS. <i>Journal of the Magnetics Society of Japan</i> , <b>1991</b> , 15, S1_73-78		
44	THEORY OF THE MAGNETO-OPTICAL PROPERTIES OF TRANSITION METALS AND RARE EARTH COMPOUNDS. Journal of the Magnetics Society of Japan, 1991, 15, S1_73-78  Electronic Structure. 2000,  Fabrication of p-Type Zns with Blue-Ag Emission by Triple-Codoping Method. Materials Research		
44 43 42	THEORY OF THE MAGNETO-OPTICAL PROPERTIES OF TRANSITION METALS AND RARE EARTH COMPOUNDS. Journal of the Magnetics Society of Japan, 1991, 15, S1_73-78  Electronic Structure. 2000,  Fabrication of p-Type Zns with Blue-Ag Emission by Triple-Codoping Method. Materials Research Society Symposia Proceedings, 2002, 719, 311  Control of Valence States for ZnO and ZnS with a Wide-Band Gap by a Codoping Method. Materials Research Society Symposia Proceedings, 2002, 719, 8331  Electronic structure and electric field gradient calculations for the Zr2Ni intermetallic compound.		
44 43 42 41	THEORY OF THE MAGNETO-OPTICAL PROPERTIES OF TRANSITION METALS AND RARE EARTH COMPOUNDS. Journal of the Magnetics Society of Japan, 1991, 15, S1_73-78  Electronic Structure. 2000,  Fabrication of p-Type Zns with Blue-Ag Emission by Triple-Codoping Method. Materials Research Society Symposia Proceedings, 2002, 719, 311  Control of Valence States for ZnO and ZnS with a Wide-Band Gap by a Codoping Method. Materials Research Society Symposia Proceedings, 2002, 719, 8331  Electronic structure and electric field gradient calculations for the Zr2Ni intermetallic compound. International Journal of Materials Research, 2009, 100, 1239-1241	4	
44 43 42 41 40	THEORY OF THE MAGNETO-OPTICAL PROPERTIES OF TRANSITION METALS AND RARE EARTH COMPOUNDS. Journal of the Magnetics Society of Japan, 1991, 15, S1_73-78  Electronic Structure. 2000,  Fabrication of p-Type Zns with Blue-Ag Emission by Triple-Codoping Method. Materials Research Society Symposia Proceedings, 2002, 719, 311  Control of Valence States for ZnO and ZnS with a Wide-Band Gap by a Codoping Method. Materials Research Society Symposia Proceedings, 2002, 719, 8331  Electronic structure and electric field gradient calculations for the Zr2Ni intermetallic compound. International Journal of Materials Research, 2009, 100, 1239-1241  The Standard ASW Method. Lecture Notes in Physics, 2012, 5-44	0.5	

36	ELECTRONIC STRUCTURE STUDIES ON TRANSITION METAL GLASSES CONTAINING HAFNIUM AND YTTRIUM. <b>1985</b> , 971-976
35	Special Semiconducting Materials. <b>1986</b> , 355-395
34	On the Electronic Structure of Calaverite. <b>1988</b> , 139-141
33	Optical Reflectivity of Glassy PdDBi Alloys. <b>1988</b> , 313-316
32	X-Ray Photoelectron Spectroscopy on Amorphous Cux Te100₪ and Nix Te100₪. <b>1988</b> , 277-280
31	References. <b>1989</b> , 563-592
30	AB-Initio Calculated Optical Properties of [001] (GaAs)n-(AlAs)n Superlattices. <i>NATO ASI Series Series B: Physics</i> , <b>1989</b> , 359-365
29	Cluster Interactions and Thermodynamic Properties of Al-Transition Metal alloys. <b>1989</b> , 515-519
28	Band Structure Calculation and Tunneling Measurements in (BEDT-TTF)2X (X= I3, IAuI). 1990, 211-220
27	Computer Applications to Materials Science and Engineering. <b>1991</b> , 81-108
26	RECENT PROGRESS IN ELECTRONIC STRUCTURE CALCULATIONS FOR DEFECTS IN METALS. <b>1991</b> , 269-274
25	Systematics in the electronic structure of amorphous transition metal/tin alloys. 1991, 107-110
24	The Influence of Magnetism and Structure on Transport Properties and Interlayer Coupling of Systems in Reduced Dimensions. <i>NATO ASI Series Series B: Physics</i> , <b>1993</b> , 155-164
23	FIRST-PRINCIPLES STUDY ON THE PHASE STABILITY OF Au-Pd ALLOYS. <b>1994</b> , 255-258
22	Magnetic Structure in Transition-Metal Compounds. <b>1994</b> , 389-395
21	Local Density Functional and Strong On-Site Correlations: The Electronic Structure of La2CuO4. <i>NATO ASI Series Series B: Physics</i> , <b>1995</b> , 525-548
20	The Role of Computational Molecular and Material Science for the Chemical Industry. <b>1996</b> , 148-158
19	A Novel Full Potential Contracted Plane Wave- (FCPW-) Method for Electronic Structure Calculations on Complex Materials. <i>NATO ASI Series Series B: Physics</i> , <b>1996</b> , 347-353

Multiple Scattering Theory Applied to XMCD Spectra in Molecule-Based Magnets. **1997**, 461-466

17	Electronic Structure and Magnetism of Itinerant 5f Ferromagnets URhSi and URhGe. <b>1999</b> , 487-498		
16	<i>Ab-Initio</i> Computations of Electronic, Transport, and Related Properties of Chromium Disilicide (CrSi<sub>2</sub>). <i>Journal of Modern Physics</i> , <b>2018</b> , 09, 2457-2472	0.5	
15	Einleitung. <b>1983</b> , 1-13		
14	Introduction. <b>2007</b> , 1-4		
13	The Standard ASW Method. <b>2007</b> , 5-45		
12	Envelope Functions and Structure Constants. <b>2007</b> , 47-115		
11	Hydrogen Trapping and Storage in the Group IVB-VIB Transition Metal Carbides. <i>Materials and Design</i> , <b>2022</b> , 214, 110399	8.1	3
10	Polymorphism of boron phosphide: theoretical investigation and experimental assessment. <i>Journal of Materials Chemistry C</i> , <b>2022</b> , 10, 3937-3943	7.1	1
9	Modification of the Atomic and Electronic Structures of Palladium as a Result of Hydrogen Dissolution. <i>Physics of the Solid State</i> , <b>2021</b> , 63, 1267-1275	0.8	
8	Zero-temperature transition between antiferromagnetic and ferromagnetic states driven by varying chemical composition in hydrogenated U2(Ni1\( \text{Ni1}\( \text{WFex}\)). <i>Physical Review B</i> , <b>2022</b> , 105,	3.3	О
7	Electronic structure and magnetic properties investigation of cubic Fe3O4. <i>Materials Today: Proceedings</i> , <b>2022</b> ,	1.4	O
6	Light induced ultrafast magnetization dynamics in metallic compounds. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2022</b> , 169596	2.8	1
5	The metal-insulator transitions of VO 2 : A band theoretical approach. <b>2002</b> , 514, 650-704		41
4	The vanadium Magn[] phases V n O 2 n -1 . <b>2004</b> , 516, 475-510		1
3	Electronic structure calculations for inhomogeneous systems: Interfaces, surfaces, and nanocontacts. <i>Annalen Der Physik</i> , <b>2008</b> , 520, 525-560	2.6	
2	Entangled origins of the nonmagnetic states of U and Fe atoms in hydrogenated UFeGe. 2023, 7,		О
1	Role of Hydride Formation in Electrocatalysis for Sustainable Chemical Transformations. <b>2023</b> , 13, 454	1-4551	O