Rudolf Zeller

List of Publications by Year in Descending Order

107 papers	5,401 citations	38 h-index	72 g-index
107 ext. papers	5,595 ext. citations	3.2 avg, IF	5.02 L-index

#	Paper	IF	Citations
107	KKRnano: Quantum Description of Skyrmions in Chiral B20 Magnets **2021**, 191-205		
106	Complex magnetism of B20-MnGe: from spin-spirals, hedgehogs to monopoles. *Journal of Physics Condensed Matter*, **2019**, 31, 485801	1.8	8
105	Towards Accurate and Large-Scale Density-Functional Calculations with the KorringaKohnRostoker Method. *Springer Proceedings in Physics*, **2018**, 313-317	0.2	
104	Structure of the high-entropy alloy Al CrFeCoNi: fcc versus bcc. *Journal of Alloys and Compounds*, **2017**, 715, 454-459	5.7	61
103	Local Energies and Energy Fluctuations Applied to the High Entropy Alloy CrFeCoNi. *Journal of the Physical Society of Japan*, **2017**, 86, 114704	1.5	9
102	Addressing Materials Science Challenges Using GPU-accelerated POWER8 Nodes. *Lecture Notes in Computer Science*, **2016**, 77-89	0.9	1
101	The Korringa-Kohn-Rostoker method with projection potentials: exact result for the density. *Journal of Physics Condensed Matter*, **2015**, 27, 306301	1.8	3
100	Systematic study of the exchange interactions in Gd-doped GaN containing N interstitials, O interstitials, or Ga vacancies. *Physical Review B*, **2015**, 92,	3.3	14
99	Dirac Green function for angular projection potentials. *Journal of Physics Condensed Matter*, **2015**, 27, 465201	1.8	
98	First-principles study of magnetic interactions in 3d transition metal-doped phase-change materials. *Physical Review B*, **2014**, 90,	3.3	17
97	Large scale supercell calculations for forces around substitutional defects in NiTi. *Physica Status Solidi (B): Basic Research*, **2014**, 251, 2048-2054	1.3	4
96	Hubbard U calculations for gap states in dilute magnetic semiconductors. *Journal of Physics Condensed Matter*, **2014**, 26, 274202	1.8	1
95	Recent Advances in the Korringa-Kohn-Rostoker Green Function Method. *EPJ Web of Conferences*, **2014**, 78, 05002	0.3	
94	Projection potentials and angular momentum convergence of total energies in the full-potential Korringa-Kohn-Rostoker method. *Journal of Physics Condensed Matter*, **2013**, 25, 105505	1.8	5
93	Preconditioning systems arising from the KKR Green function method using block-circulant matrices. *Linear Algebra and Its Applications*, **2012**, 436, 436-446	0.9	4
92	Lifetime reduction of surface states at Cu, Ag, and Au(111) caused by impurity scattering. *Physical Review B*, **2012**, 86,	3.3	8
91	Role of vacancies in metal-insulator transitions of crystalline phase-change materials. *Nature Materials*, **2012**, 11, 952-6	27	220

90	Massively parallel density functional calculations for thousands of atoms: KKRnano. *Physical Review B*, **2012**, 85,	3.3	29
89	Superparamagnetism in Gd-doped GaN induced by Ga-vacancy clustering. *Physical Review B*, **2012**, 86,	3.3	22
88	Linear Scaling for Metallic Systems by the Korringa-Kohn-Rostoker Multiple-Scattering Method. *Challenges and Advances in Computational Chemistry and Physics*, **2011**, 475-505	0.7	
87	Linear-scaling total-energy calculations with the tight-binding Korringa-Kohn-Rostoker Green function method. *Philosophical Magazine*, **2008**, 88, 2807-2815	1.6	4
86	Improving the charge density normalization in Korringa□Kohn□Rostoker Green-function calculations. *Journal of Physics Condensed Matter*, **2008**, 20, 035220	1.8	12
85	Towards a linear-scaling algorithm for electronic structure calculations with the tight-binding Korringa□Kohn□Rostoker Green function method. *Journal of Physics Condensed Matter*, **2008**, 20, 294215	1.8	24
84	Noncollinear magnetism of Cr and Mn nanoclusters on Ni(111): Changing the magnetic configuration atom by atom. *Physical Review B*, **2007**, 75,	3.3	25
83	Vacancy complexes with oversized impurities in Si and Ge. *Physical Review B*, **2005**, 71,	3.3	57
82	Lloyd□ formula in multiple-scattering calculations with finite temperature. *Journal of Physics Condensed Matter*, **2005**, 17, 5367-5379	1.8	8
81	Influence of spin-orbit coupling on the transport properties of magnetic tunnel junctions. *Physical Review B*, **2005**, 72,	3.3	18
80	Cd-vacancy and Cd-interstitial complexes in Si and Ge. *Physical Review B*, **2004**, 70,	3.3	12
79	Spin-dependent transport in ferromagnet/semiconductor/ferromagnet junctions: a fully relativistic approach. *Journal of Physics Condensed Matter*, **2004**, 16, S5579-S5586	1.8	12
78	Effect of the spin-orbit interaction on the band gap of half metals. *Physical Review B*, **2004**, 69,	3.3	104
77	An elementary derivation of Lloyd□s formula valid for full-potential multiple-scattering theory. *Journal of Physics Condensed Matter*, **2004**, 16, 6453-6468	1.8	28
76	Full-potential KKR calculations for vacancies in Al: Screening effect and many-body interactions. *Physical Review B*, **2004**, 70,	3.3	24
75	Full-potential KKR calculations for MgO and divalent impurities in MgO. *Physical Review B*, **2002**, 66,	3.3	21
74	Effects of resonant interface states on tunneling magnetoresistance. *Physical Review B*, **2002**, 65,	3.3	121
73	Ballistic spin injection from Fe(001) into ZnSe and GaAs. *Physical Review B*, **2002**, 65,	3.3	72

72	Electronic structure of Fe/semiconductor/Fe(001) tunnel junctions. *Physical Review B*, **2002**, 66,	3.3	22
71	Orbital magnetism of transition-metal adatoms and clusters on the Ag and Au(001) surfaces. *Physical Review B*, **2002**, 65,	3.3	62
70	Magnetic 4d monoatomic rows on Ag vicinal surfaces. *Physical Review B*, **2001**, 64,	3.3	31
69	Cd hyperfine fields at the bcc Fe/Co interface. *Physical Review B*, **2001**, 64,	3.3	4
68	Lattice relaxations and hyperfine fields of heavy impurities in Fe. *Physical Review B*, **2000**, 62, 452-460	3.3	30
67	Scanning tunneling spectra of impurities in the Fe(001) surface. *Physical Review B*, **2000**, 62, 11118-11125	3.3	27
66	Magnetic nanostructures on the fcc Fe/Cu(100) surface. *Physical Review B*, **2000**, 61, 2356-2361	3.3	11
65	Imperfect magnetic nanostructures on a Ag(001) surface. *Physical Review B*, **1999**, 59, 1681-1684	3.3	38
64	First-principles calculations for vacancy formation energies in Cu and Al; non-local effect beyond the LSDA and lattice distortion. *Computational Materials Science*, **1999**, 14, 56-61	3.2	48
63	Full-potential KKR calculations for metals and semiconductors. *Physical Review B*, **1999**, 60, 5202-5210	3.3	103
62	Conceptual and computational advances in multiple-scattering electronic-structure calculations. *Computational Materials Science*, **1998**, 10, 373-380	3.2	1
61	Full-potential spin-polarized relativistic Korringa-Kohn-Rostoker method implemented and applied to bcc Fe, fcc Co, and fcc Ni. *Physical Review B*, **1998**, 58, 10236-10247	3.3	120
60	Magnetic properties of 4d impurities on the (001) surfaces of nickel and iron. *Physical Review B*, **1998**, 57, 84-87	3.3	11
59	Short-period oscillations in photoemission from Cu films on Co(100). *Physical Review B*, **1998**, 57, R696-R699	3.3	26
58	Total energy and magnetic moments in disordered FexCu1-x alloys. *Physical Review B*, **1998**, 57, 5213-5219	3.3	62
57	Interface reflectivities and quantum-well states in magnetic multilayers. *Physical Review B*, **1998**, 58, 13721-13733	3.3	18
56	Hyperfine Fields of sp Impurities on Ni and Fe Surfaces. *Physical Review Letters*, **1998**, 81, 1505-1508	7.4	18
55	Hyperfine fields of probe atoms on the (001) surface of Ni. *The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties*, **1998**, 78, 435-440		4

54	Lattice distortion in Cu-based dilute alloys: A first-principles study by the KKR Green-function method. *Physical Review B*, **1997**, 55, 4157-4167	3.3	113
53	Relationship between magnetism, topology, and reactivity of Rh clusters. *Physical Review B*, **1997**, 56, 8849-8854	3.3	79
52	Screened KKR-Green's-function method for layered systems. *Physical Review B*, **1997**, 55, 10074-10080	3.3	61
51	Evaluation of the screened Korringa-Kohn-Rostoker method for accurate and large-scale electronic-structure calculations. *Physical Review B*, **1997**, 55, 9400-9408	3.3	61
50	Ab initio study of structural distortion and its influence on the magnetic properties of metallic dilute alloys. *Computational Materials Science*, **1997**, 8, 131-135	3.2	20
49	Ab initio calculations of interaction energies of magnetic layers in noble metals: Co/Cu(100). *Physical Review B*, **1996**, 53, 9092-9107	3.3	56
48	Local-density-functional calculations for defect interactions in Al. *Physical Review B*, **1996**, 53, 8971-8974	3.3	38
47	Accurate evaluation of the interstitial KKR Green function. *Physical Review B*, **1996**, 54, 4531-4539	3.3	5
46	Magnetism of 3d, 4d, and 5d transition-metal impurities on Pd(001) and Pt(001) surfaces. *Physical Review B*, **1996**, 53, 2121-2125	3.3	118
45	Interaction energies of 111In perturbed-angular-correlation probes with 3d and 4sp impurities in Ag, Pd, and Rh. *Physical Review B*, **1996**, 53, 5247-5251	3.3	6
44	Magnetic behavior of transition-metal impurities in alkali-earth metals. *Physical Review B*, **1995**, 51, 11473-11478	3.3	7
43	Fermi-Dirac distribution in ab initio Green's-function calculations. *Physical Review B*, **1995**, 52, 11502-11508	3.3	98
42	Theory and convergence properties of the screened Korringa-Kohn-Rostoker method. *Physical Review B*, **1995**, 52, 8807-8812	3.3	277
41	Magnetic impurities in simple metals. *Physica Scripta*, **1994**, 50, 445-448	2.6	1
40	Influence of the magnetic-layer thickness on the interlayer exchange coupling: Competition between oscillation periods. *Physical Review B*, **1994**, 50, 13058-13061	3.3	66
39	Can 5d and sp impurities be magnetic?. *Physical Review Letters*, **1993**, 71, 629-632	7.4	25
38	Green's function calculations of the hyperfine interaction for impurities in metals andfor metallic interfaces. *Hyperfine Interactions*, **1993**, 78, 341-359	0.8	11
37	Calculation of the residual resistivity and the thermoelectric power of sp impurities in silver. *Physical Review B*, **1992**, 46, 15761-15766	3.3	15

36	Interaction energies of perturbed-angular-correlation probes with impurities in Ag and Pd. *Physical Review B*, **1992**, 45, 12202-12209	3.3	14
35	Theoretical study of the anisotropic hyperfine interaction of Cu atoms close to 3d impurities. *Physical Review B*, **1992**, 45, 7841-7849	3.3	1
34	Local spin moments of transition-metal impurities in monovalent simple-metal hosts. *Physical Review B*, **1992**, 46, 10858-10865	3.3	35
33	Calculation of shape-truncation functions for Voronoi polyhedra. *Journal of Physics Condensed Matter*, **1991**, 3, 7599-7606	1.8	42
32	Vacancy-solute interactions in Cu, Ni, Ag, and Pd. *Physical Review B*, **1991**, 43, 9487-9497	3.3	56
31	Local perturbation and induced magnetization originating from 3d impurities in Pd. *Physical Review B*, **1991**, 43, 9558-9568	3.3	25
30	Parametrization of the electronic structure of Z+1 impurities. *Physical Review B*, **1991**, 43, 13916-13925	3.3	19
29	An efficient numerical method to calculate shape truncation functions for Wigner-Seitz atomic polyhedra. *Computer Physics Communications*, **1990**, 60, 231-238	4.2	65
28	Electric-field gradients in dilute Cu alloys: The role of the Cu d electrons. *Physical Review B*, **1990**, 42, 9336-9339	3.3	25
27	Electronic structure of Z+1 impurities in metals. *Physical Review B*, **1990**, 41, 2753-2757	3.3	24
26	Comment on "Exact eigenvalue equation for a finite and infinite collection of muffin-tin potentials". *Physical Review B*, **1990**, 41, 10224-10225	3.3	5
25	Ab initio calculations of NMR satellite data for 3d impurities in Cu. *Physical Review B*, **1989**, 39, 6334-6341	3.3	28
24	Electronic structure and magnetic properties of dilute Fe alloys with transition-metal impurities. *Physical Review B*, **1989**, 40, 8203-8212	3.3	155
23	First-principles calculation of impurity-solution energies in Cu and Ni. *Physical Review B*, **1989**, 39, 930-939	3.3	109
22	Empty-lattice test for non-muffin-tin multiple-scattering equations. *Physical Review B*, **1988**, 38, 5993-6002	3.3	19
21	Hyperfine fields of 3d and 4d impurities in nickel. *Physical Review B*, **1987**, 35, 3271-3283	3.3	308
20	Ab initio electronic structure calculations for point defects in CoAl and CoGa. *Physical Review B*, **1987**, 35, 2705-2713	3.3	24
19	Charge and magnetization perturbations around impurities in nickel. *Physical Review B*, **1987**, 35, 6911-6922	3.3	49

18	Treatment of lattice relaxations in dilute alloys within the Korringa-Kohn-Rostoker Green's-function method. *Physical Review B*, **1987**, 36, 6372-6382	3.3	33
17	Theory of F centers in the alkaline-earth oxides MgO and CaO. *Physical Review B*, **1987**, 35, 5802-5815	3.3	83
16	Electronic structure of Pd alloys. *Solid State Communications*, **1987**, 62, 735-738	1.6	34
15	Electronic structure of antistructure Co atoms and Co-vacancies in CoAl. *Solid State Communications* , **1986**, 59, 429-432	1.6	9
14	Electronic structure of substoichiometric carbides and nitrides of zirconium and niobium. *Physical Review B*, **1986**, 33, 6709-6717	3.3	40
13	Electronic structure of the carbon vacancy in NbC. *Physical Review B*, **1986**, 34, 2517-2521	3.3	28
12	Role of electron-energy losses in bremsstrahlung isochromat spectroscopy. *Physical Review B*, **1986** , 34, 5177-5183	3.3	21
11	Electronic structure of substoichiometric carbides and nitrides of titanium and vanadium. *Physical Review B*, **1986**, 33, 812-822	3.3	138
10	Studies of total density of states of metals up to 70 eV above EF. *Physical Review B*, **1985**, 32, 3597-3603	3.3	86
9	Self-consistent cluster calculations with correct embedding for3d,4d, and somespimpurities in copper. *Physical Review B*, **1984**, 29, 703-718	3.3	245
8	Bremsstrahlung isochromat spectra and density-of-states calculations for the 3d and 4d transition metals. *Physical Review B*, **1984**, 30, 6921-6930	3.3	123
7	The density and pressure of helium in bubbles in metals. *Radiation Effects*, **1983**, 78, 315-325		61
6	Electronic structure of Ni and Pd alloys. I. X-ray photoelectron spectroscopy of the valence bands. *Physical Review B*, **1983**, 27, 2145-2178	3.3	295
5	Self-consistency iterations in electronic-structure calculations. *Physical Review B*, **1983**, 28, 5462-5472	3.3	110
4	Growth of he bubbles in al during annealing. *Radiation Effects*, **1983**, 78, 327-336		23
3	Electronic structure of impurities in transition metals **1981**, 243-269		14
2	Electronic structure of magnetic impurities calculated from first principles. *Physical Review B*, **1980**, 22, 5777-5790	3.3	249
1	Variational treatment of the elastic constants of disordered materials. *Zeitschrift Fü Physik A*, **1973** , 259, 103-116		165