

Rudolf Zeller

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107
papers

5,401
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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	Hyperfine fields of 3d and 4d impurities in nickel. <i>Physical Review B</i> , 1987 , 35, 3271-3283	3.3	308
106	Electronic structure of Ni and Pd alloys. I. X-ray photoelectron spectroscopy of the valence bands. <i>Physical Review B</i> , 1983 , 27, 2145-2178	3.3	295
105	Theory and convergence properties of the screened Korringa-Kohn-Rostoker method. <i>Physical Review B</i> , 1995 , 52, 8807-8812	3.3	277
104	Electronic structure of magnetic impurities calculated from first principles. <i>Physical Review B</i> , 1980 , 22, 5777-5790	3.3	249
103	Self-consistent cluster calculations with correct embedding for 3d, 4d, and some s impurities in copper. <i>Physical Review B</i> , 1984 , 29, 703-718	3.3	245
102	Role of vacancies in metal-insulator transitions of crystalline phase-change materials. <i>Nature Materials</i> , 2012 , 11, 952-6	27	220
101	Variational treatment of the elastic constants of disordered materials. <i>Zeitschrift für Physik A</i> , 1973 , 259, 103-116		165
100	Electronic structure and magnetic properties of dilute Fe alloys with transition-metal impurities. <i>Physical Review B</i> , 1989 , 40, 8203-8212	3.3	155
99	Electronic structure of substoichiometric carbides and nitrides of titanium and vanadium. <i>Physical Review B</i> , 1986 , 33, 812-822	3.3	138
98	Bremsstrahlung isochromat spectra and density-of-states calculations for the 3d and 4d transition metals. <i>Physical Review B</i> , 1984 , 30, 6921-6930	3.3	123
97	Effects of resonant interface states on tunneling magnetoresistance. <i>Physical Review B</i> , 2002 , 65,	3.3	121
96	Full-potential spin-polarized relativistic Korringa-Kohn-Rostoker method implemented and applied to bcc Fe, fcc Co, and fcc Ni. <i>Physical Review B</i> , 1998 , 58, 10236-10247	3.3	120
95	Magnetism of 3d, 4d, and 5d transition-metal impurities on Pd(001) and Pt(001) surfaces. <i>Physical Review B</i> , 1996 , 53, 2121-2125	3.3	118
94	Lattice distortion in Cu-based dilute alloys: A first-principles study by the KKR Green-function method. <i>Physical Review B</i> , 1997 , 55, 4157-4167	3.3	113
93	Self-consistency iterations in electronic-structure calculations. <i>Physical Review B</i> , 1983 , 28, 5462-5472	3.3	110
92	First-principles calculation of impurity-solution energies in Cu and Ni. <i>Physical Review B</i> , 1989 , 39, 930-939	3.3	109
91	Effect of the spin-orbit interaction on the band gap of half metals. <i>Physical Review B</i> , 2004 , 69,	3.3	104

90	Full-potential KKR calculations for metals and semiconductors. <i>Physical Review B</i> , 1999 , 60, 5202-5210	3-3	103
89	Fermi-Dirac distribution in ab initio Green's-function calculations. <i>Physical Review B</i> , 1995 , 52, 11502-11508	3-3	98
88	Studies of total density of states of metals up to 70 eV above EF. <i>Physical Review B</i> , 1985 , 32, 3597-3603	3-3	86
87	Theory of F centers in the alkaline-earth oxides MgO and CaO. <i>Physical Review B</i> , 1987 , 35, 5802-5815	3-3	83
86	Relationship between magnetism, topology, and reactivity of Rh clusters. <i>Physical Review B</i> , 1997 , 56, 8849-8854	3-3	79
85	Ballistic spin injection from Fe(001) into ZnSe and GaAs. <i>Physical Review B</i> , 2002 , 65,	3-3	72
84	Influence of the magnetic-layer thickness on the interlayer exchange coupling: Competition between oscillation periods. <i>Physical Review B</i> , 1994 , 50, 13058-13061	3-3	66
83	An efficient numerical method to calculate shape truncation functions for Wigner-Seitz atomic polyhedra. <i>Computer Physics Communications</i> , 1990 , 60, 231-238	4-2	65
82	Orbital magnetism of transition-metal adatoms and clusters on the Ag and Au(001) surfaces. <i>Physical Review B</i> , 2002 , 65,	3-3	62
81	Total energy and magnetic moments in disordered Fe _x Cu _{1-x} alloys. <i>Physical Review B</i> , 1998 , 57, 5213-5219	3-3	62
80	Structure of the high-entropy alloy Al CrFeCoNi: fcc versus bcc. <i>Journal of Alloys and Compounds</i> , 2017 , 715, 454-459	5-7	61
79	Screened KKR-Green's-function method for layered systems. <i>Physical Review B</i> , 1997 , 55, 10074-10080	3-3	61
78	Evaluation of the screened Korringa-Kohn-Rostoker method for accurate and large-scale electronic-structure calculations. <i>Physical Review B</i> , 1997 , 55, 9400-9408	3-3	61
77	The density and pressure of helium in bubbles in metals. <i>Radiation Effects</i> , 1983 , 78, 315-325		61
76	Vacancy complexes with oversized impurities in Si and Ge. <i>Physical Review B</i> , 2005 , 71,	3-3	57
75	Ab initio calculations of interaction energies of magnetic layers in noble metals: Co/Cu(100). <i>Physical Review B</i> , 1996 , 53, 9092-9107	3-3	56
74	Vacancy-solute interactions in Cu, Ni, Ag, and Pd. <i>Physical Review B</i> , 1991 , 43, 9487-9497	3-3	56
73	Charge and magnetization perturbations around impurities in nickel. <i>Physical Review B</i> , 1987 , 35, 6911-6922	3-3	49

72	First-principles calculations for vacancy formation energies in Cu and Al; non-local effect beyond the LSDA and lattice distortion. <i>Computational Materials Science</i> , 1999 , 14, 56-61	3.2	48
71	Calculation of shape-truncation functions for Voronoi polyhedra. <i>Journal of Physics Condensed Matter</i> , 1991 , 3, 7599-7606	1.8	42
70	Electronic structure of substoichiometric carbides and nitrides of zirconium and niobium. <i>Physical Review B</i> , 1986 , 33, 6709-6717	3.3	40
69	Imperfect magnetic nanostructures on a Ag(001) surface. <i>Physical Review B</i> , 1999 , 59, 1681-1684	3.3	38
68	Local-density-functional calculations for defect interactions in Al. <i>Physical Review B</i> , 1996 , 53, 8971-8974	3.3	38
67	Local spin moments of transition-metal impurities in monovalent simple-metal hosts. <i>Physical Review B</i> , 1992 , 46, 10858-10865	3.3	35
66	Electronic structure of Pd alloys. <i>Solid State Communications</i> , 1987 , 62, 735-738	1.6	34
65	Treatment of lattice relaxations in dilute alloys within the Korringa-Kohn-Rostoker Green's-function method. <i>Physical Review B</i> , 1987 , 36, 6372-6382	3.3	33
64	Magnetic 4d monoatomic rows on Ag vicinal surfaces. <i>Physical Review B</i> , 2001 , 64,	3.3	31
63	Lattice relaxations and hyperfine fields of heavy impurities in Fe. <i>Physical Review B</i> , 2000 , 62, 452-460	3.3	30
62	Massively parallel density functional calculations for thousands of atoms: KKRnano. <i>Physical Review B</i> , 2012 , 85,	3.3	29
61	An elementary derivation of Lloyd's formula valid for full-potential multiple-scattering theory. <i>Journal of Physics Condensed Matter</i> , 2004 , 16, 6453-6468	1.8	28
60	Ab initio calculations of NMR satellite data for 3d impurities in Cu. <i>Physical Review B</i> , 1989 , 39, 6334-6341	3.3	28
59	Electronic structure of the carbon vacancy in NbC. <i>Physical Review B</i> , 1986 , 34, 2517-2521	3.3	28
58	Scanning tunneling spectra of impurities in the Fe(001) surface. <i>Physical Review B</i> , 2000 , 62, 11118-11125	3.3	27
57	Short-period oscillations in photoemission from Cu films on Co(100). <i>Physical Review B</i> , 1998 , 57, R696-R699	3.3	26
56	Noncollinear magnetism of Cr and Mn nanoclusters on Ni(111): Changing the magnetic configuration atom by atom. <i>Physical Review B</i> , 2007 , 75,	3.3	25
55	Can 5d and sp impurities be magnetic?. <i>Physical Review Letters</i> , 1993 , 71, 629-632	7.4	25

54	Local perturbation and induced magnetization originating from 3d impurities in Pd. <i>Physical Review B</i> , 1991 , 43, 9558-9568	3.3	25
53	Electric-field gradients in dilute Cu alloys: The role of the Cu d electrons. <i>Physical Review B</i> , 1990 , 42, 9336-9339	3.3	25
52	Towards a linear-scaling algorithm for electronic structure calculations with the tight-binding Korringa-Kohn-Rostoker Green function method. <i>Journal of Physics Condensed Matter</i> , 2008 , 20, 294215	1.8	24
51	Full-potential KKR calculations for vacancies in Al: Screening effect and many-body interactions. <i>Physical Review B</i> , 2004 , 70,	3.3	24
50	Electronic structure of Z+1 impurities in metals. <i>Physical Review B</i> , 1990 , 41, 2753-2757	3.3	24
49	Ab initio electronic structure calculations for point defects in CoAl and CoGa. <i>Physical Review B</i> , 1987 , 35, 2705-2713	3.3	24
48	Growth of he bubbles in al during annealing. <i>Radiation Effects</i> , 1983 , 78, 327-336		23
47	Superparamagnetism in Gd-doped GaN induced by Ga-vacancy clustering. <i>Physical Review B</i> , 2012 , 86,	3.3	22
46	Electronic structure of Fe/semiconductor/Fe(001) tunnel junctions. <i>Physical Review B</i> , 2002 , 66,	3.3	22
45	Full-potential KKR calculations for MgO and divalent impurities in MgO. <i>Physical Review B</i> , 2002 , 66,	3.3	21
44	Role of electron-energy losses in bremsstrahlung isochromat spectroscopy. <i>Physical Review B</i> , 1986 , 34, 5177-5183	3.3	21
43	Ab initio study of structural distortion and its influence on the magnetic properties of metallic dilute alloys. <i>Computational Materials Science</i> , 1997 , 8, 131-135	3.2	20
42	Parametrization of the electronic structure of Z+1 impurities. <i>Physical Review B</i> , 1991 , 43, 13916-13925	3.3	19
41	Empty-lattice test for non-muffin-tin multiple-scattering equations. <i>Physical Review B</i> , 1988 , 38, 5993-6003	3.3	19
40	Influence of spin-orbit coupling on the transport properties of magnetic tunnel junctions. <i>Physical Review B</i> , 2005 , 72,	3.3	18
39	Interface reflectivities and quantum-well states in magnetic multilayers. <i>Physical Review B</i> , 1998 , 58, 13721-13733	3.3	18
38	Hyperfine Fields of sp Impurities on Ni and Fe Surfaces. <i>Physical Review Letters</i> , 1998 , 81, 1505-1508	7.4	18
37	First-principles study of magnetic interactions in 3d transition metal-doped phase-change materials. <i>Physical Review B</i> , 2014 , 90,	3.3	17

36	Calculation of the residual resistivity and the thermoelectric power of sp impurities in silver. <i>Physical Review B</i> , 1992 , 46, 15761-15766	3.3	15
35	Systematic study of the exchange interactions in Gd-doped GaN containing N interstitials, O interstitials, or Ga vacancies. <i>Physical Review B</i> , 2015 , 92,	3.3	14
34	Interaction energies of perturbed-angular-correlation probes with impurities in Ag and Pd. <i>Physical Review B</i> , 1992 , 45, 12202-12209	3.3	14
33	Electronic structure of impurities in transition metals 1981 , 243-269		14
32	Improving the charge density normalization in Korringa-Kohn-Rostoker Green-function calculations. <i>Journal of Physics Condensed Matter</i> , 2008 , 20, 035220	1.8	12
31	Cd-vacancy and Cd-interstitial complexes in Si and Ge. <i>Physical Review B</i> , 2004 , 70,	3.3	12
30	Spin-dependent transport in ferromagnet/semiconductor/ferromagnet junctions: a fully relativistic approach. <i>Journal of Physics Condensed Matter</i> , 2004 , 16, S5579-S5586	1.8	12
29	Magnetic nanostructures on the fcc Fe/Cu(100) surface. <i>Physical Review B</i> , 2000 , 61, 2356-2361	3.3	11
28	Magnetic properties of 4d impurities on the (001) surfaces of nickel and iron. <i>Physical Review B</i> , 1998 , 57, 84-87	3.3	11
27	Green's function calculations of the hyperfine interaction for impurities in metals and for metallic interfaces. <i>Hyperfine Interactions</i> , 1993 , 78, 341-359	0.8	11
26	Local Energies and Energy Fluctuations Applied to the High Entropy Alloy CrFeCoNi. <i>Journal of the Physical Society of Japan</i> , 2017 , 86, 114704	1.5	9
25	Electronic structure of antistructure Co atoms and Co-vacancies in CoAl. <i>Solid State Communications</i> , 1986 , 59, 429-432	1.6	9
24	Complex magnetism of B20-MnGe: from spin-spirals, hedgehogs to monopoles. <i>Journal of Physics Condensed Matter</i> , 2019 , 31, 485801	1.8	8
23	Lifetime reduction of surface states at Cu, Ag, and Au(111) caused by impurity scattering. <i>Physical Review B</i> , 2012 , 86,	3.3	8
22	Lloyd's formula in multiple-scattering calculations with finite temperature. <i>Journal of Physics Condensed Matter</i> , 2005 , 17, 5367-5379	1.8	8
21	Magnetic behavior of transition-metal impurities in alkali-earth metals. <i>Physical Review B</i> , 1995 , 51, 114733-11478	3.3	11
20	Interaction energies of 111In perturbed-angular-correlation probes with 3d and 4sp impurities in Ag, Pd, and Rh. <i>Physical Review B</i> , 1996 , 53, 5247-5251	3.3	6
19	Projection potentials and angular momentum convergence of total energies in the full-potential Korringa-Kohn-Rostoker method. <i>Journal of Physics Condensed Matter</i> , 2013 , 25, 105505	1.8	5

18	Accurate evaluation of the interstitial KKR Green function. <i>Physical Review B</i> , 1996 , 54, 4531-4539	3.3	5
17	Comment on "Exact eigenvalue equation for a finite and infinite collection of muffin-tin potentials". <i>Physical Review B</i> , 1990 , 41, 10224-10225	3.3	5
16	Large scale supercell calculations for forces around substitutional defects in NiTi. <i>Physica Status Solidi (B): Basic Research</i> , 2014 , 251, 2048-2054	1.3	4
15	Preconditioning systems arising from the KKR Green function method using block-circulant matrices. <i>Linear Algebra and Its Applications</i> , 2012 , 436, 436-446	0.9	4
14	Linear-scaling total-energy calculations with the tight-binding Korringa-Kohn-Rostoker Green function method. <i>Philosophical Magazine</i> , 2008 , 88, 2807-2815	1.6	4
13	Cd hyperfine fields at the bcc Fe/Co interface. <i>Physical Review B</i> , 2001 , 64,	3.3	4
12	Hyperfine fields of probe atoms on the (001) surface of Ni. <i>The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties</i> , 1998 , 78, 435-440		4
11	The Korringa-Kohn-Rostoker method with projection potentials: exact result for the density. <i>Journal of Physics Condensed Matter</i> , 2015 , 27, 306301	1.8	3
10	Hubbard U calculations for gap states in dilute magnetic semiconductors. <i>Journal of Physics Condensed Matter</i> , 2014 , 26, 274202	1.8	1
9	Conceptual and computational advances in multiple-scattering electronic-structure calculations. <i>Computational Materials Science</i> , 1998 , 10, 373-380	3.2	1
8	Magnetic impurities in simple metals. <i>Physica Scripta</i> , 1994 , 50, 445-448	2.6	1
7	Theoretical study of the anisotropic hyperfine interaction of Cu atoms close to 3d impurities. <i>Physical Review B</i> , 1992 , 45, 7841-7849	3.3	1
6	Addressing Materials Science Challenges Using GPU-accelerated POWER8 Nodes. <i>Lecture Notes in Computer Science</i> , 2016 , 77-89	0.9	1
5	Towards Accurate and Large-Scale Density-Functional Calculations with the Korringa-Kohn-Rostoker Method. <i>Springer Proceedings in Physics</i> , 2018 , 313-317	0.2	
4	Recent Advances in the Korringa-Kohn-Rostoker Green Function Method. <i>EPJ Web of Conferences</i> , 2014 , 78, 05002	0.3	
3	Dirac Green function for angular projection potentials. <i>Journal of Physics Condensed Matter</i> , 2015 , 27, 465201	1.8	
2	Linear Scaling for Metallic Systems by the Korringa-Kohn-Rostoker Multiple-Scattering Method. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2011 , 475-505	0.7	
1	KKRnano: Quantum Description of Skyrmions in Chiral B20 Magnets 2021 , 191-205		

