Rudolf Zeller

List of Publications by Year
in descending order

107	5,881	87723 38	74018 75
papers	citations	h-index	g-index

107	107	107	2998
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Hyperfine fields of 3dand 4dimpurities in nickel. Physical Review B, 1987, 35, 3271-3283.	1.1	337
2	Electronic structure of Ni and Pd alloys. I. X-ray photoelectron spectroscopy of the valence bands. Physical Review B, 1983, 27, 2145-2178.	1.1	316
3	Theory and convergence properties of the screened Korringa-Kohn-Rostoker method. Physical Review B, 1995, 52, 8807-8812.	1.1	312
4	Role of vacancies in metalâ€“insulator transitions of crystalline phase-change materials. Nature Materials, 2012, 11, 952-956.	13.3	258
5	Electronic structure of magnetic impurities calculated from first principles. Physical Review B, 1980, 22, 5777-5790.	1.1	255
6	Self-consistent cluster calculations with correct embedding for3d,4d, and somespimpurities in copper. Physical Review B, 1984, 29, 703-718.	1.1	250
7	Variational treatment of the elastic constants of disordered materials. Zeitschrift FÃ¼r Physik A, 1973, 259, 103-116.	0.9	181
8	Electronic structure and magnetic properties of dilute Fe alloys with transition-metal impurities. Physical Review B, 1989, 40, 8203-8212.	1.1	159
9	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.	1.1	152
10	Electronic structure of substoichiometric carbides and nitrides of titanium and vanadium. Physical Review B, 1986, 33, 812-822.	1.1	144
11	Self-consistency iterations in electronic-structure calculations. Physical Review B, 1983, 28, 5462-5472.	1.1	137
12	Bremsstrahlung isochromat spectra and density-of-states calculations for the3dand4dtransition metals. Physical Review B, 1984, 30, 6921-6930.	1.1	130
13	Effects of resonant interface states on tunneling magnetoresistance. Physical Review B, 2002, 65, .	1.1	130
14	Lattice distortion in Cu-based dilute alloys: A first-principles study by the KKR Green-function method. Physical Review B, 1997, 55, 4157-4167.	1.1	129
15	Magnetism of 3d, 4d, and 5dtransition-metal impurities on Pd(001) and Pt(001) surfaces. Physical Review B, 1996, 53, 2121-2125.	1.1	125
16	Full-potential KKR calculations for metals and semiconductors. Physical Review B, 1999, 60, 5202-5210.	1.1	112
17	Effect of the spin-orbit interaction on the band gap of half metals. Physical Review B, 2004, 69, .	1.1	111
18	First-principles calculation of impurity-solution energies in Cu and Ni. Physical Review B, 1989, 39, 930-939.	1.1	110

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19	Fermi-Dirac distribution inab initioGreenâ€™s-function calculations. Physical Review B, 1995, 52, 11502-11508.	1.1	104
20	Studies of total density of states of metals up to 70 eV aboveEF. Physical Review B, 1985, 32, 3597-3603.	1.1	87
21	Structure of the high-entropy alloy Al CrFeCoNi: fcc versus bcc. Journal of Alloys and Compounds, 2017, 715, 454-459.	2.8	87
22	Total energy and magnetic moments in disorderedFexCu1â^'xalloys. Physical Review B, 1998, 57, 5213-5219.	1.1	86
23	Theory ofFcenters in the alkaline-earth oxides MgO and CaO. Physical Review B, 1987, 35, 5802-5815.	1.1	85
24	Relationship between magnetism, topology, and reactivity of Rh clusters. Physical Review B, 1997, 56, 8849-8854.	1.1	81
25	Ballistic spin injection from Fe(001) into ZnSe and GaAs. Physical Review B, 2002, 65, .	1.1	81
26	An efficient numerical method to calculate shape truncation functions for Wigner-Seitz atomic polyhedra. Computer Physics Communications, 1990, 60, 231-238.	3.0	74
27	Influence of the magnetic-layer thickness on the interlayer exchange coupling: Competition between oscillation periods. Physical Review B, 1994, 50, 13058-13061.	1.1	67
28	The density and pressure of helium in bubbles in metals. Radiation Effects, 1983, 78, 315-325.	0.4	65
29	Screened KKR-Green's-function method for layered systems. Physical Review B, 1997, 55, 10074-10080.	1.1	64
30	Orbital magnetism of transition-metal adatoms and clusters on the Ag and Au(001) surfaces. Physical Review B, 2002, 65, .	1.1	64
31	Evaluation of the screened Korringa-Kohn-Rostoker method for accurate and large-scale electronic-structure calculations. Physical Review B, 1997, 55, 9400-9408.	1.1	63
32	Vacancy complexes with oversized impurities in Si and Ge. Physical Review B, 2005, 71, .	1.1	63
33	Vacancy-solute interactions in Cu, Ni, Ag, and Pd. Physical Review B, 1991, 43, 9487-9497.	1.1	58
34	Ab initiocalculations of interaction energies of magnetic layers in noble metals: Co/Cu(100). Physical Review B, 1996, 53, 9092-9107.	1.1	58
35	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.	1.4	53
36	Charge and magnetization perturbations around impurities in nickel. Physical Review B, 1987, 35, 6911-6922.	1.1	51

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37	Calculation of shape-truncation functions for Voronoi polyhedra. Journal of Physics Condensed Matter, 1991, 3, 7599-7606.	0.7	48
38	Electronic structure of substoichiometric carbides and nitrides of zirconium and niobium. Physical Review B, 1986, 33, 6709-6717.	1.1	46
39	Local-density-functional calculations for defect interactions in Al. Physical Review B, 1996, 53, 8971-8974.	1.1	39
40	Imperfect magnetic nanostructures on a Ag(001) surface. Physical Review B, 1999, 59, 1681-1684.	1.1	38
41	Treatment of lattice relaxations in dilute alloys within the Korringa-Kohn-Rostoker Greenâ€™s-function method. Physical Review B, 1987, 36, 6372-6382.	1.1	37
42	Electronic structure of Pd alloys. Solid State Communications, 1987, 62, 735-738.	0.9	35
43	Local spin moments of transition-metal impurities in monovalent simple-metal hosts. Physical Review B, 1992, 46, 10858-10865.	1.1	35
44	Magnetic4dmonoatomic rows on Ag vicinal surfaces. Physical Review B, 2001, 64, .	1.1	33
45	Massively parallel density functional calculations for thousands of atoms: KKRnano. Physical Review B, 2012, 85, .	1.1	32
46	Electronic structure of the carbon vacancy in NbC. Physical Review B, 1986, 34, 2517-2521.	1.1	31
47	Lattice relaxations and hyperfine fields of heavy impurities in Fe. Physical Review B, 2000, 62, 452-460.	1.1	31
48	An elementary derivation of LloydÂs formula valid for full-potential multiple-scattering theory. Journal of Physics Condensed Matter, 2004, 16, 6453-6468.	0.7	31
49	Ab initiocalculations of NMR satellite data for 3dimpurities in Cu. Physical Review B, 1989, 39, 6334-6341.	1.1	29
50	Scanning tunneling spectra of impurities in the Fe(001) surface. Physical Review B, 2000, 62, 11118-11125.	1.1	29
51	Electronic structure of Z+1 impurities in metals. Physical Review B, 1990, 41, 2753-2757.	1.1	27
52	Can 5dandspimpurities be magnetic?. Physical Review Letters, 1993, 71, 629-632.	2.9	27
53	Short-period oscillations in photoemission from Cu films on Co(100). Physical Review B, 1998, 57, R696-R699.	1.1	27
54	Electric-field gradients in dilute Cu alloys: The role of the Cudelectrons. Physical Review B, 1990, 42, 9336-9339.	1.1	26

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55	Local perturbation and induced magnetization originating from 3dimpurities in Pd. Physical Review B, 1991, 43, 9558-9568.	1.1	26
56	Full-potential KKR calculations for vacancies inAl: Screening effect and many-body interactions. Physical Review B, 2004, 70, .	1.1	26
57	Noncollinear magnetism of Cr and Mn nanoclusters on Ni(111): Changing the magnetic configuration atom by atom. Physical Review B, 2007, 75, .	1.1	26
58	Towards a linear-scaling algorithm for electronic structure calculations with the tight-binding Korringaâ€“Kohnâ€“Rostoker Green function method. Journal of Physics Condensed Matter, 2008, 20, 294215.	0.7	26
59	Abinitioelectronic structure calculations for point defects in CoAl and CoGa. Physical Review B, 1987, 35, 2705-2713.	1.1	25
60	Growth of he bubbles in al during annealing. Radiation Effects, 1983, 78, 327-336.	0.4	23
61	Electronic structure of Fe/semiconductor/Fe(001) tunnel junctions. Physical Review B, 2002, 66, .	1.1	23
62	Superparamagnetism in Gd-doped GaN induced by Ga-vacancy clustering. Physical Review B, 2012, 86, .	1.1	23
63	Role of electron-energy losses in bremsstrahlung isochromat spectroscopy. Physical Review B, 1986, 34, 5177-5183.	1.1	22
64	Full-potential KKR calculations for MgO and divalent impurities in MgO. Physical Review B, 2002, 66, .	1.1	22
65	Local Energies and Energy Fluctuations â€” Applied to the High Entropy Alloy CrFeCoNi. Journal of the Physical Society of Japan, 2017, 86, 114704.	0.7	22
66	Parametrization of the electronic structure ofZ+1 impurities. Physical Review B, 1991, 43, 13916-13925.	1.1	20
67	Ab initio study of structural distortion and its influence on the magnetic properties of metallic dilute alloys. Computational Materials Science, 1997, 8, 131-135.	1.4	20
68	Interface reflectivities and quantum-well states in magnetic multilayers. Physical Review B, 1998, 58, 13721-13733.	1.1	20
69	Influence of spin-orbit coupling on the transport properties of magnetic tunnel junctions. Physical Review B, 2005, 72, .	1.1	20
70	Empty-lattice test for non-muffin-tin multiple-scattering equations. Physical Review B, 1988, 38, 5993-6002.	1.1	19
71	Hyperfine Fields ofspImpurities on Ni and Fe Surfaces. Physical Review Letters, 1998, 81, 1505-1508.	2.9	19
72	Improving the charge density normalization in Korringaâ€“Kohnâ€“Rostoker Green-function calculations. Journal of Physics Condensed Matter, 2008, 20, 035220.	0.7	19

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73	First-principles study of magnetic interactions in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:math>transition metal-doped phase-change materials. Physical Review B, 2014, 90, .	1.1	18
74	Calculation of the residual resistivity and the thermoelectric power ofspimpurities in silver. Physical Review B, 1992, 46, 15761-15766.	1.1	16
75	Systematic study of the exchange interactions in Gd-doped GaN containing N interstitials, O interstitials, or Ga vacancies. Physical Review B, 2015, 92, .	1.1	16
76	Electronic structure of impurities in transition metals. , 1981, , 243-269.		15
77	Interaction energies of perturbed-angular-correlation probes with impurities in Ag and Pd. Physical Review B, 1992, 45, 12202-12209.	1.1	14
78	Magnetic properties of4dimpurities on the (001) surfaces of nickel and iron. Physical Review B, 1998, 57, 84-87.	1.1	14
79	Cd-vacancy andCd-interstitial complexes inSiandGe. Physical Review B, 2004, 70, .	1.1	14
80	Spin-dependent transport in ferromagnet/semiconductor/ferromagnet junctions: a fully relativistic approach. Journal of Physics Condensed Matter, 2004, 16, S5579-S5586.	0.7	13
81	Complex magnetism of B20-MnGe: from spin-spirals, hedgehogs to monopoles. Journal of Physics Condensed Matter, 2019, 31, 485801.	0.7	12
82	Green's function calculations of the hyperfine interaction for impurities in metals andfor metallic interfaces. Hyperfine Interactions, 1993, 78, 341-359.	0.2	11
83	Magnetic nanostructures on the fcc Fe/Cu(100) surface. Physical Review B, 2000, 61, 2356-2361.	1.1	11
84	Lifetime reduction of surface states at Cu, Ag, and Au(111) caused by impurity scattering. Physical Review B, 2012, 86, .	1.1	10
85	Electronic structure of antistructure Co atoms and Co-vacancies in CoAl. Solid State Communications, 1986, 59, 429-432.	0.9	9
86	Magnetic behavior of transition-metal impurities in alkali-earth metals. Physical Review B, 1995, 51, 11473-11478.	1.1	8
87	Lloydâ€™s formula in multiple-scattering calculations with finite temperature. Journal of Physics Condensed Matter, 2005, 17, 5367-5379.	0.7	8
88	Interaction energies ofIn111perturbed-angular-correlation probes with 3dand 4spimpurities in Ag, Pd, and Rh. Physical Review B, 1996, 53, 5247-5251.	1.1	6
89	Projection potentials and angular momentum convergence of total energies in the full-potential Korringaâ€“Kohnâ€“Rostoker method. Journal of Physics Condensed Matter, 2013, 25, 105505.	0.7	6
90	Comment on â€˜â€˜Exact eigenvalue equation for a finite and infinite collection of muffin-tin potentialsâ€™â€™. Physical Review B, 1990, 41, 10224-10225.	1.1	5

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91	Accurate evaluation of the interstitial KKR Green function. Physical Review B, 1996, 54, 4531-4539.	1.1	5
92	Large scale supercell calculations for forces around substitutional defects in NiTi. Physica Status Solidi (B): Basic Research, 2014, 251, 2048-2054.	0.7	5
93	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.	0.6	4
94	Cd hyperfine fields at the bcc Fe/Co interface. Physical Review B, 2001, 64, .	1.1	4
95	Linear-scaling total-energy calculations with the tight-binding Korringa-Kohn-Rostoker Green function method. Philosophical Magazine, 2008, 88, 2807-2815.	0.7	4
96	Preconditioning systems arising from the KKR Green function method using block-circulant matrices. Linear Algebra and Its Applications, 2012, 436, 436-446.	0.4	4
97	The Korringaâ€“Kohnâ€“Rostoker method with projection potentials: exact result for the density. Journal of Physics Condensed Matter, 2015, 27, 306301.	0.7	3
98	Theoretical study of the anisotropic hyperfine interaction of Cu atoms close to 3dimpurities. Physical Review B, 1992, 45, 7841-7849.	1.1	1
99	Magnetic impurities in simple metals. Physica Scripta, 1994, 50, 445-448.	1.2	1
100	Conceptual and computational advances in multiple-scattering electronic-structure calculations. Computational Materials Science, 1998, 10, 373-380.	1.4	1
101	HubbardUcalculations for gap states in dilute magnetic semiconductors. Journal of Physics Condensed Matter, 2014, 26, 274202.	0.7	1
102	Addressing Materials Science Challenges Using GPU-accelerated POWER8 Nodes. Lecture Notes in Computer Science, 2016, , 77-89.	1.0	1
103	Recent Advances in the Korringa-Kohn-Rostoker Green Function Method. EPJ Web of Conferences, 2014, 78, 05002.	0.1	0
104	Dirac Green function for angular projection potentials. Journal of Physics Condensed Matter, 2015, 27, 465201.	0.7	0
105	Towards Accurate and Large-Scale Density-Functional Calculations with the Korringaâ€“Kohnâ€“Rostoker Method. Springer Proceedings in Physics, 2018, , 313-317.	0.1	0
106	KKRnano: Quantum Description of Skyrmions in Chiral B20 Magnets. , 2021, , 191-205.		0
107	Linear Scaling for Metallic Systems by the Korringa-Kohn-Rostoker Multiple-Scattering Method. Challenges and Advances in Computational Chemistry and Physics, 2011, , 475-505.	0.6	0