Karlheinz Schwarz

List of Publications by Year
in descending order

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60	13,378	109321	128289
papers	citations	35 h-index	60 g-index

61	61	61	10486
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Full-potential, linearized augmented plane wave programs for crystalline systems. Computer Physics Communications, 1990, 59, 399-415.	7.5	3,005
2	Electronic structure calculations of solids using the WIEN2k package for material sciences. Computer Physics Communications, 2002, 147, 71-76.	7.5	1,582
3	WIEN2k: An APW+lo program for calculating the properties of solids. Journal of Chemical Physics, 2020, 152, 074101.	3.0	1,185
4	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
5	Solid state calculations using WIEN2k. Computational Materials Science, 2003, 28, 259-273.	3.0	1,008
6	Efficient linearization of the augmented plane-wave method. Physical Review B, 2001, 64, .	3.2	914
7	Hybrid exchange-correlation energy functionals for strongly correlated electrons: Applications to transition-metal monoxides. Physical Review B, 2006, 74, .	3.2	309
8	DFT calculations of solids with LAPW and WIEN2k. Journal of Solid State Chemistry, 2003, 176, 319-328.	2.9	306
9	Performance on molecules, surfaces, and solids of the Wu-Cohen GGA exchange-correlation energy functional. Physical Review B, 2007, 75, .	3.2	306
10	Itinerant metamagnetism in YCO2. Journal of Physics F: Metal Physics, 1984, 14, L129-L134.	1.6	300
11	First-Principles Calculation of the Electric Field Gradient ofLi3N. Physical Review Letters, 1985, 54, 1192-1195.	7.8	289
12	Determination of the Nuclear Quadrupole Moment of57Fe. Physical Review Letters, 1995, 75, 3545-3548.	7.8	251
13	Charge distribution and electric-field gradients inYBa2Cu3O7â^'x. Physical Review B, 1990, 42, 2051-2061.	3.2	248
14	Electronic structure of fcc Th: Spin-orbit calculation with6p1/2local orbital extension. Physical Review B, 2001, 64, .	3.2	219
15	Density functional theory investigation of the geometric and spintronic structure ofh-BN/Ni(111) in view of photoemission and STM experiments. Physical Review B, 2003, 68, .	3.2	179
16	Magnetic structure and electric-field gradients of uranium dioxide: Anab initiostudy. Physical Review B, 2004, 69, .	3.2	155
17	Single-Layer Model of the Hexagonal Boron Nitride Nanomesh on the Rh(111) Surface. Physical Review Letters, 2007, 98, 106802.	7.8	147
18	Electronic structure of solids with WIEN2k. Molecular Physics, 2010, 108, 3147-3166.	1.7	133

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19	Theory of orientation-sensitive near-edge fine-structure core-level spectroscopy. Physical Review B, 1999, 59, 12807-12814.	3.2	120
20	Electric-field-gradient calculations for systems with large extended-core-state contributions. Physical Review B, 1992, 46, 1321-1325.	3.2	108
21	DFT Study of the Role of Al³⁺ in the Fast Ion-Conductor Li_{7â€“3x}Al³⁺_xLa₃Zr₂O₁₂ Garnet. Chemistry of Materials, 2014, 26, 2617-2623.	9.7	108
22	Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, 10881-10905.	3.3	108
23	Competing structural instabilities in the ferroelectric Aurivillius compoundSrBi2Ta2O9. Physical Review B, 2004, 70, .	3.2	104
24	Correlation Induced Paramagnetic Ground State in FeAl. Physical Review Letters, 2001, 87, 196401.	7.8	95
25	Magnetic and half-metallic properties of the full-Heusler alloys Co2TiX(X=Al,Ga;Si,Ge,Sn;Sb). Journal of Applied Physics, 2005, 97, 10C307.	2.5	81
26	Epitaxial growth of hexagonal boron nitride on Ag(111). Physical Review B, 2010, 82, .	3.2	75
27	Temperature and composition dependence of crystal structures and magnetic and electronic properties of the double perovskites<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>La</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn> Physical Review B, 2010, 82, .	3.2	74
28	The orientation-dependent simulation of ELNES. Ultramicroscopy, 2000, 83, 9-16.	1.9	70
29	First-principles calculations of strontium on Si(001). Physical Review B, 2004, 69, .	3.2	62
30	Scissors implementation within length-gauge formulations of the frequency-dependent nonlinear optical response of semiconductors. Physical Review B, 2005, 72, .	3.2	58
31	Multiple instabilities in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Bi</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">Ti</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>12</mml:mn></mml:msub></mml:mrow></mml:math>: A ferroelectric beyond the soft-mode paradigm. Physical Review B, 2008, 77, .	3.2	53
32	Partial core hole screening in the Cu L 3 edge. European Physical Journal B, 2001, 21, 363-367.	1.5	51
33	On the existence of non-nuclear maxima in simple metals. Journal of Chemical Physics, 2002, 117, 8030-8035.	3.0	39
34	Investigation of the Optical and Excitonic Properties of the Visible Light-Driven Photocatalytic BiVO₄ Material. Chemistry of Materials, 2017, 29, 3380-3386.	6.7	38
35	Materials design of solid electrolytes. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 3497-3497.	7.1	35
36	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>PBE</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math>calculat of the Jahn-Teller effect in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Pr</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2008, 77, .	3.2	35

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37	Density functional calculations on the charge-ordered and valence-mixed modification of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>YBaFe</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2009, 79, .	3.2	35
38	Short-range magnetic order and temperature-dependent properties of cupric oxide. Journal of Physics Condensed Matter, 2010, 22, 045502.	1.8	35
39	Magnetic structure and orbital ordering inBaCoO3from first-principles calculations. Physical Review B, 2004, 70, .	3.2	33
40	Polarization-Dependent Raman Characterization of Stibnite (Sb[sub 2]S[sub 3]). AIP Conference Proceedings, 2010, , .	0.4	30
41	Electric field gradients in cuprates: Does LDA+U give the correct charge distribution?. International Journal of Quantum Chemistry, 2005, 101, 550-556.	2.0	27
42	Shortcomings of meta-GGA functionals when describing magnetism. Physical Review B, 2020, 102, .	3.2	27
43	Evidence for magnetic clusters inBaCoO3. Physical Review B, 2004, 70, .	3.2	25
44	Force calculation for orbital-dependent potentials with FP-(L)APW+lo basis sets. Computer Physics Communications, 2008, 179, 784-790.	7.5	25
45	Adsorption of small gold clusters on the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>h</mml:mi></mml:math>-BN/Rh(111) nanomesh. Physical Review B, 2012, 86, .	3.2	24
46	Geometric Frustration, Electronic Instabilities, and Charge Singlets inY2Nb2O7. Physical Review Letters, 2004, 93, 216403.	7.8	21
47	Iterative diagonalization in augmented plane wave based methods in electronic structure calculations. Journal of Computational Physics, 2010, 229, 453-460.	3.8	21
48	Density functional theory simulations of B K and N K NEXAFS spectra of h-BN/transition metal(111) interfaces. Journal of Physics Condensed Matter, 2009, 21, 104210.	1.8	19
49	How Close Are the Slater and Beckeâ€“Roussel Potentials in Solids?. Journal of Chemical Theory and Computation, 2015, 11, 4717-4726.	5.3	17
50	Chemistry of La on the Si(001) surface from first principles. Physical Review B, 2004, 70, .	3.2	16
51	Ab initiostudy of stabilization of the misfit layer compound<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mtext>PbS</mml:mtext></mml:mrow></mml:mrow></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review B, 2010, 82, .	3.2	16
52	Quantum oscillations of the superconductor LaRu2P2: Comparable mass enhancementÎ»â‰ˆ1in Ru and Fe phosphides. Physical Review B, 2011, 84, .	3.2	11
53	Light emission from direct band gap germanium containing split-interstitial defects. Physical Review B, 2021, 103, .	3.2	11
54	Ising-type behavior in the antiferromagnetic phase of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Ba</mml:mi><mml:mi mathvariant="normal">Co</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>from first principles. Physical Review B, 2007, 76, .	3.2	9

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55	Obituary for Walter Kohn (1923â€“2016). Computation, 2016, 4, 40.	2.0	3
56	MÃ¶ssbauer study of LaNiSn and NdNiSn compounds and their deuterides. Journal of Radioanalytical and Nuclear Chemistry, 2005, 266, 553-556.	1.5	2
57	Computation: A New Open Access Journal of Computational Chemistry, Computational Biology and Computational Engineering. Computation, 2013, 1, 27-30.	2.0	1
58	Special Issue â€œ50th Anniversary of the Kohnâ€“Sham Theoryâ€”Advances in Density Functional Theoryâ€• Computation, 2016, 4, 45.	2.0	1
59	Challenges for Theory and Computation. Computation, 2017, 5, 49.	2.0	1
60	Frontispiece: Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, .	3.3	1