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	Light emission from direct band gap germanium containing split-interstitial defects. Physical Review B, 2021, 103, .	3.2	11
2	Shortcomings of meta-GGA functionals when describing magnetism. Physical Review B, 2020, 102, .	3.2	27
3	WIEN2k: An APW+lo program for calculating the properties of solids. Journal of Chemical Physics, 2020, 152, 074101.	3.0	1,185
4	Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, 10881-10905.	3.3	108
5	Frontispiece: Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, .	3.3	1
6	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
7	Challenges for Theory and Computation. Computation, 2017, 5, 49.	2.0	1
8	Obituary for Walter Kohn (1923â€“2016). Computation, 2016, 4, 40.	2.0	3
9	Special Issue â€œ50th Anniversary of the Kohnâ€“Sham Theoryâ€”Advances in Density Functional Theoryâ€. Computation, 2016, 4, 45.	2.0	1
10	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
11	How Close Are the Slater and Beckeâ€“Roussel Potentials in Solids?. Journal of Chemical Theory and Computation, 2015, 11, 4717-4726.	5.3	17
12	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.	8.7	108
13	Computation: A New Open Access Journal of Computational Chemistry, Computational Biology and Computational Engineering. Computation, 2013, 1, 27-30.	2.0	1
14	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
15	Quantum oscillations of the superconductor LaRu2P2: Comparable mass enhancementÎ»â‰ˆ1in Ru and Fe phosphides. Physical Review B, 2011, 84, .	3.2	11
16	Iterative diagonalization in augmented plane wave based methods in electronic structure calculations. Journal of Computational Physics, 2010, 229, 453-460.	3.8	21
17	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> Physical Review B, 2010, 82, .	3.2	16
18	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

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19	Epitaxial growth of hexagonal boron nitride on Ag(111). Physical Review B, 2010, 82, .	3.2	75
20	Polarization-Dependent Raman Characterization of Stibnite (Sb[sub 2]S[sub 3]). AIP Conference Proceedings, 2010, , .	0.4	30
21	Short-range magnetic order and temperature-dependent properties of cupric oxide. Journal of Physics Condensed Matter, 2010, 22, 045502.	1.8	35
22	Electronic structure of solids with WIEN2k. Molecular Physics, 2010, 108, 3147-3166.	1.7	133
23	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
24	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:m Physical Review B, 2009, 79, .	3.2	35
25	Force calculation for orbital-dependent potentials with FP-(L)APW+lo basis sets. Computer Physics Communications, 2008, 179, 784-790.	7.5	25
26	<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>.	3.2	35
27	<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	3.2	53
28	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
29	Performance on molecules, surfaces, and solids of the Wu-Cohen GGA exchange-correlation energy functional. Physical Review B, 2007, 75, .	3.2	306
30	Single-Layer Model of the Hexagonal Boron Nitride Nanomesh on the Rh(111) Surface. Physical Review Letters, 2007, 98, 106802.	7.8	147
31	Hybrid exchange-correlation energy functionals for strongly correlated electrons: Applications to transition-metal monoxides. Physical Review B, 2006, 74, .	3.2	309
32	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
33	MÃ¶ssbauer study of LaNiSn and NdNiSn compounds and their deuterides. Journal of Radioanalytical and Nuclear Chemistry, 2005, 266, 553-556.	1.5	2
34	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
35	Scissors implementation within length-gauge formulations of the frequency-dependent nonlinear optical response of semiconductors. Physical Review B, 2005, 72, .	3.2	58
36	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

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37	Geometric Frustration, Electronic Instabilities, and Charge Singlets inY2Nb2O7. Physical Review Letters, 2004, 93, 216403.	7.8	21
38	First-principles calculations of strontium on Si(001). Physical Review B, 2004, 69, .	3.2	62
39	Magnetic structure and electric-field gradients of uranium dioxide: Anab initiostudy. Physical Review B, 2004, 69, .	3.2	155
40	Chemistry of La on the Si(001) surface from first principles. Physical Review B, 2004, 70, .	3.2	16
41	Competing structural instabilities in the ferroelectric Aurivillius compoundSrBi2Ta2O9. Physical Review B, 2004, 70, .	3.2	104
42	Evidence for magnetic clusters inBaCoO3. Physical Review B, 2004, 70, .	3.2	25
43	Magnetic structure and orbital ordering inBaCoO3from first-principles calculations. Physical Review B, 2004, 70, .	3.2	33
44	DFT calculations of solids with LAPW and WIEN2k. Journal of Solid State Chemistry, 2003, 176, 319-328.	2.9	306
45	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
46	Solid state calculations using WIEN2k. Computational Materials Science, 2003, 28, 259-273.	3.0	1,008
47	On the existence of non-nuclear maxima in simple metals. Journal of Chemical Physics, 2002, 117, 8030-8035.	3.0	39
48	Electronic structure calculations of solids using the WIEN2k package for material sciences. Computer Physics Communications, 2002, 147, 71-76.	7.5	1,582
49	Efficient linearization of the augmented plane-wave method. Physical Review B, 2001, 64, .	3.2	914
50	Partial core hole screening in the Cu L 3 edge. European Physical Journal B, 2001, 21, 363-367.	1.5	51
51	Electronic structure of fcc Th: Spin-orbit calculation with6p1/2local orbital extension. Physical Review B, 2001, 64, .	3.2	219
52	Correlation Induced Paramagnetic Ground State in FeAl. Physical Review Letters, 2001, 87, 196401.	7.8	95
53	The orientation-dependent simulation of ELNES. Ultramicroscopy, 2000, 83, 9-16.	1.9	70
54	Theory of orientation-sensitive near-edge fine-structure core-level spectroscopy. Physical Review B, 1999, 59, 12807-12814.	3.2	120

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55	Determination of the Nuclear Quadrupole Moment of57Fe. Physical Review Letters, 1995, 75, 3545-3548.	7.8	251
56	Electric-field-gradient calculations for systems with large extended-core-state contributions. Physical Review B, 1992, 46, 1321-1325.	3.2	108
57	Full-potential, linearized augmented plane wave programs for crystalline systems. Computer Physics Communications, 1990, 59, 399-415.	7.5	3,005
58	Charge distribution and electric-field gradients inYBa2Cu3O7â^'x. Physical Review B, 1990, 42, 2051-2061.	3.2	248
59	First-Principles Calculation of the Electric Field Gradient ofLi3N. Physical Review Letters, 1985, 54, 1192-1195.	7.8	289
60	Itinerant metamagnetism in YCO2. Journal of Physics F: Metal Physics, 1984, 14, L129-L134.	1.6	300