Mark Van Schilfgaarde

List of Publications by Year
in descending order

109 papers	16,589 citations	28274 55 h-index	24982 109 g-index
109 all docs	109 docs citations	109 times ranked	16542 citing authors

#	Article	IF	Citations
1	Supercurrent decay in ballistic magnetic Josephson junctions. Npj Computational Materials, 2022, 8, .	8.7	9
2	Role of nematicity in controlling spin fluctuations and superconducting <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>T</mml:mi><mml:mi>c</mml:mi></mml:msub></mml:ma in bulk FeSe. Physical Review B, 2022, 105, .	3.2	4
3	Real- and momentum-space description of the excitons in bulk and monolayer chromium tri-halides. Npj 2D Materials and Applications, 2022, 6, .	7.9	12
4	Electronic and optical properties of crystalline nitrogen versus black phosphorus: A comparative first-principles study. Physical Review B, 2022, 105, .	3.2	3
5	Real-space representation of the quasiparticle self-consistent <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m self-energy and its application to defect calculations. Physical Review B, 2022, 105, .	3.2	2
6	Electronic Structure Correspondence of Singlet-Triplet Scale Separation in Strained Sr2RuO4. Applied Sciences (Switzerland), 2021, 11, 508.	2.5	4
7	Electronic Origin of Tc in Bulk and Monolayer FeSe. Symmetry, 2021, 13, 169.	2.2	9
8	Optical response and band structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LiCoO</mml:mi><mml:mn>2</mml:mn></mml:msub></m including electron-hole interaction effects. Physical Review B, 2021, 104, .	3.2	18
9	Ultrafast Carrier and Lattice Dynamics in Plasmonic Nanocrystalline Copper Sulfide Films. Laser and Photonics Reviews, 2021, 15, 2000346.	8.7	9
10	Electronic structure of chromium trihalides beyond density functional theory. Physical Review B, 2021, 104, .	3.2	18
11	Importance of charge self-consistency in first-principles description of strongly correlated systems. Npj Computational Materials, 2021, 7, .	8.7	13
12	Questaal: A package of electronic structure methods based on the linear muffin-tin orbital technique. Computer Physics Communications, 2020, 249, 107065.	7.5	82
13	Controlling Tc through Band Structure and Correlation Engineering in Collapsed and Uncollapsed Phases of Iron Arsenides. Physical Review Letters, 2020, 124, 237001.	7.8	11
14	Electronâ€“phonon-driven three-dimensional metallicity in an insulating cuprate. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 6409-6416.	7.1	18
15	Role of the lattice in the light-induced insulator-to-metal transition in vanadium dioxide. Physical Review Research, 2020, 2, .	3.6	9
16	Anisotropic Plasmonic CuS Nanocrystals as a Natural Electronic Material with Hyperbolic Optical Dispersion. ACS Nano, 2019, 13, 6550-6560.	14.6	30
17	Impact of nonparabolic electronic band structure on the optical and transport properties of photovoltaic materials. Physical Review B, 2019, 99, .	3.2	60
18	Evening out the spin and charge parity to increase $${T}_{c}$$ in $${{m{Sr}}}_{2}{{m{RuO}}}_{4}$$. Communications Physics, 2019, 2, .	5.3	26

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19	Origin of Pronounced Nonlinear Band Gap Behavior in Leadâ€“Tin Hybrid Perovskite Alloys. Chemistry of Materials, 2018, 30, 3920-3928.	6.7	166
20	Magnetic properties of chromium-doped Ni80Fe20 thin films. Journal of Magnetism and Magnetic Materials, 2018, 460, 193-202.	2.3	7
21	Acoustic phonon lifetimes limit thermal transport in methylammonium lead iodide. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 11905-11910.	7.1	81
22	Rotational Cation Dynamics in Metal Halide Perovskites: Effect on Phonons and Material Properties. Journal of Physical Chemistry Letters, 2018, 9, 5987-5997.	4.6	68
23	Metal-Insulator Transition in Copper Oxides Induced by Apex Displacements. Physical Review X, 2018, 8, .	8.9	11
24	Dynamic symmetry breaking and spin splitting in metal halide perovskites. Physical Review B, 2018, 98, .	3.2	52
25	Effect of ladder diagrams on optical absorption spectra in a quasiparticle self-consistent <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="italic">GW</mml:mi></mml:math> framework. Physical Review Materials, 2018, 2, .	2.4	45
26	Organic Cation Rotation and Immobilization in Pure and Mixed Methylammonium Lead-Halide Perovskites. Journal of the American Chemical Society, 2017, 139, 4068-4074.	13.7	114
27	Perspective: Theory and simulation of hybrid halide perovskites. Journal of Chemical Physics, 2017, 146, 220901.	3.0	111
28	Indirect to direct bandgap transition in methylammonium lead halide perovskite. Energy and Environmental Science, 2017, 10, 509-515.	30.8	318
29	Spontaneous Octahedral Tilting in the Cubic Inorganic Cesium Halide Perovskites CsSnX₃ and CsPbX₃ (X = F, Cl, Br, I). Journal of Physical Chemistry Letters, 2017, 8, 4720-4726.	4.6	186
30	Emergent Properties of an Organic Semiconductor Driven by its Molecular Chirality. ACS Nano, 2017, 11, 8329-8338.	14.6	136
31	The magnetic, electrical and structural properties of copper-permalloy alloys. Journal of Magnetism and Magnetic Materials, 2017, 442, 45-52.	2.3	11
32	Self-energies in itinerant magnets: A focus on Fe and Ni. Physical Review B, 2017, 95, .	3.2	39
33	Quasi-particle electronic band structure and alignment of the V-VI-VII semiconductors SbSI, SbSBr, and SbSeI for solar cells. Applied Physics Letters, 2016, 108, .	3.3	59
34	Research Update: Relativistic origin of slow electron-hole recombination in hybrid halide perovskite solar cells. APL Materials, 2016, 4, .	5.1	178
35	Direct Observation of Dynamic Symmetry Breaking above Room Temperature in Methylammonium Lead Iodide Perovskite. ACS Energy Letters, 2016, 1, 880-887.	17.4	221
36	Computational Screening of All Stoichiometric Inorganic Materials. CheM, 2016, 1, 617-627.	11.7	115

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37	First-principles treatment of Mott insulators: linearized QSGW+DMFT approach. Npj Quantum Materials, 2016, 1, .	5.2	54
38	Computational materials design of crystalline solids. Chemical Society Reviews, 2016, 45, 6138-6146.	38.1	105
39	What Is Moving in Hybrid Halide Perovskite Solar Cells?. Accounts of Chemical Research, 2016, 49, 528-535.	15.6	385
40	Experimental and theoretical optical properties of methylammonium lead halide perovskites. Nanoscale, 2016, 8, 6317-6327.	5.6	385
41	Direct method for calculating temperature-dependent transport properties. Physical Review B, 2015, 91, .	3.2	57
42	Band-filling effect on magnetic anisotropy using a Green's function method. Physical Review B, 2015, 92, .	3.2	42
43	Lattice dynamics and vibrational spectra of the orthorhombic, tetragonal, and cubic phases of methylammonium lead iodide. Physical Review B, 2015, 92, .	3.2	452
44	Cubic Perovskite Structure of Black Formamidinium Lead Iodide, Î±-[HC(NH₂)₂]PbI₃, at 298 K. Journal of Physical Chemistry Letters, 2015, 6, 3209-3212.	4.6	457
45	Ionic transport in hybrid lead iodide perovskite solar cells. Nature Communications, 2015, 6, 7497.	12.8	2,154
46	Reversible Hydration of CH₃NH₃PbI₃ in Films, Single Crystals, and Solar Cells. Chemistry of Materials, 2015, 27, 3397-3407.	6.7	1,133
47	Influence of Intermolecular Interactions on the Reorganization Energy of Charge Transfer between Surface-Attached Dye Molecules. Journal of Physical Chemistry C, 2015, 119, 24337-24341.	3.1	14
48	Role of microstructure in the electronâ€“hole interaction of hybrid lead halide perovskites. Nature Photonics, 2015, 9, 695-701.	31.4	226
49	Real-Time Observation of Organic Cation Reorientation in Methylammonium Lead Iodide Perovskites. Journal of Physical Chemistry Letters, 2015, 6, 3663-3669.	4.6	322
50	Ferroelectric materials for solar energy conversion: photoferroics revisited. Energy and Environmental Science, 2015, 8, 838-848.	30.8	333
51	Models of charge pair generation in organic solar cells. Physical Chemistry Chemical Physics, 2015, 17, 2311-2325.	2.8	158
52	Band alignment of the hybrid halide perovskites CH₃NH₃PbCl₃, CH₃NH₃PbBr₃and CH₃NH₃PbI₃. Materials Horizons, 2015, 2, 228-231.	12.2	238
53	Atomistic Origins of High-Performance in Hybrid Halide Perovskite Solar Cells. Nano Letters, 2014, 14, 2584-2590.	9.1	2,068
54	Molecular ferroelectric contributions to anomalous hysteresis in hybrid perovskite solar cells. APL Materials, 2014, 2, .	5.1	481

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55	Influence of Chemical Structure on the Charge Transfer State Spectrum of a Polymer:Fullerene Complex. Journal of Physical Chemistry C, 2014, 118, 8253-8261.	3.1	61
56	Relativistic quasiparticle self-consistent electronic structure of hybrid halide perovskite photovoltaic absorbers. Physical Review B, 2014, 89, .	3.2	612
57	Criteria for improving the properties of ZnGeAs₂ solar cells. Progress in Photovoltaics: Research and Applications, 2013, 21, 906-917.	8.1	13
58	Effects of alloying and strain on the magnetic properties of Fe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>16</mml:mn></mml:msub></mml:math>N<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2013, 88, .	3.2	72
59	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Fe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>4</mml:mn><mml:mo>+</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>Se<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow /></mml:msub></mml:math>	3.2	11
60	Effect of correlations on electronic structure and transport across (001) Fe/MgO/Fe junctions. Physical Review B, 2012, 85, .	3.2	11
61	Doping-induced metallicity and coexistence of magnetic subsystems in K2Fe4+xSe5. Solid State Communications, 2012, 152, 1846-1849.	1.9	1
62	Spin filtering with EuO: Insight from the complex band structure. Physical Review B, 2012, 85, .	3.2	24
63	Low-energy coherent Stoner-like excitations inCaFe2As2. Physical Review B, 2011, 83, .	3.2	12
64	On the Chemical Origin of the Gap Bowing in (GaAs)1â^'x Ge2x Alloys: A Combined DFTâ€“QSGW Study. Nanoscale Research Letters, 2010, 5, 469-477.	5.7	22
65	Thin film tandem photovoltaic cell from II-IV-V chalcopyrites. Applied Physics Letters, 2010, 96, 143503.	3.3	18
66	Fusion of the LAPW and LMTO methods: The augmented plane wave plus muffin-tin orbital method. Physical Review B, 2010, 81, .	3.2	90
67	Impact ionization rates for Si, GaAs, InAs, ZnS, and GaN in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>approximation. Physical Review B, 2010, 81, .	3.2	34
68	Spin wave dispersion based on the quasiparticle self-consistentGWmethod: NiO, MnO and Î±-MnAs. Journal of Physics Condensed Matter, 2008, 20, 295214.	1.8	55
69	Reversal of Spin Polarization inFe/GaAs(001) Driven by Resonant Surface States: First-Principles Calculations. Physical Review Letters, 2007, 99, 196603.	7.8	75
70	Electronic structure of rare-earth nitrides using theLSDA+Uapproach: Importance of allowing4forbitals to break the cubic crystal symmetry. Physical Review B, 2007, 75, .	3.2	332
71	Tunneling Anisotropic Magnetoresistance Driven by Resonant Surface States: First-Principles Calculations on an Fe(001) Surface. Physical Review Letters, 2007, 98, 046601.	7.8	93
72	Breakdown of a gold nanowire between electrodes. Nanotechnology, 2007, 18, 424002.	2.6	7

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73	Quasiparticle self-consistent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>method: A basis for the independent-particle approximation. Physical Review B, 2007, 76, .	3.2	364
74	Quasiparticle self-consistentGWmethod: a short summary. Journal of Physics Condensed Matter, 2007, 19, 365236.	1.8	24
75	Quasiparticle self-consistent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>method applied to localized<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>4</mml:mn><mml:mi>f</mml:mi></mml:mrow></mml:math>electron systems. Physical Review B, 2007, 76, .	3.2	91
76	AbÂInitioPrediction of Conduction Band Spin Splitting in Zinc Blende Semiconductors. Physical Review Letters, 2006, 96, 086405.	7.8	193
77	Adequacy of approximations inGWtheory. Physical Review B, 2006, 74, .	3.2	149
78	Ab initiotight-binding LMTO method for nonequilibrium electron transport in nanosystems. Physical Review B, 2005, 71, .	3.2	81
79	Experimental and theoretical investigation of the structural, chemical, electronic, and high frequency dielectric properties of barium cadmium tantalateâ€“based ceramics. Journal of Applied Physics, 2005, 97, 014105.	2.5	14
80	Theoretical study of environmental dependence of oxygen vacancy formation in CeO2. Applied Physics Letters, 2005, 87, 141917.	3.3	56
81	A First Principles Alloy Scattering Approach for Monte Carlo Hole Mobility Calculations. Journal of Computational Electronics, 2004, 3, 351-354.	2.5	1
82	Electronic properties of alkali-metal loaded zeolites: Supercrystal Mott insulators. Physical Review B, 2004, 69, .	3.2	27
83	All-Electron Self-ConsistentGWApproximation: Application to Si, MnO, and NiO. Physical Review Letters, 2004, 93, 126406.	7.8	475
84	Spin lifetimes of electrons injected into GaAs and GaN. Applied Physics Letters, 2003, 83, 1761-1763.	3.3	109
85	Theoretical and Experimental Study of Barium Zinc-Cadmium Tantalate-based Microwave Dielectrics. Materials Research Society Symposia Proceedings, 2003, 783, 471.	0.1	1
86	All-electron GW approximation with the mixed basis expansion based on the full-potential LMTO method. Solid State Communications, 2002, 121, 461-465.	1.9	168
87	GW quasiparticle band structure of CaB6. Journal of Physics and Chemistry of Solids, 2002, 63, 1595-1597.	4.0	13
88	Pressure-Induced Invar Effect in Fe-Ni Alloys. Physical Review Letters, 2001, 86, 4851-4854.	7.8	78
89	Atomistic simulations on the tensile debonding of an aluminumâ€“silicon interface. Journal of the Mechanics and Physics of Solids, 2000, 48, 2183-2212.	4.8	157
90	Direct gap in ordered silicon carbon alloys. Applied Physics Letters, 1999, 75, 3153-3155.	3.3	7

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91	Origin of the Invar effect in ironâ€“nickel alloys. Nature, 1999, 400, 46-49.	27.8	487
92	Bandstructure effect on high-field transport in GaN and GaAlN. Applied Physics Letters, 1997, 71, 1999-2001.	3.3	53
93	Effective masses and valence-band splittings in GaN and AlN. Physical Review B, 1997, 56, 7363-7375.	3.2	226
94	Theory of Oscillatory Exchange Coupling in Fe/(V,Cr) and Fe/(Cr,Mn). Physical Review Letters, 1995, 74, 4063-4066.	7.8	50
95	Pressure Dependence of III-V Schottky Barriers: A Critical Test of Theories for Fermi Level Pinning. Physical Review Letters, 1994, 73, 581-584.	7.8	19
96	InTlSb: An infrared detector material?. Applied Physics Letters, 1993, 62, 1857-1859.	3.3	47
97	Oscillatory exchange coupling: RKKY or quantum-well mechanism?. Physical Review Letters, 1993, 71, 3870-3873.	7.8	69
98	Simplified first principles approach to exchange coupling in magnetic multilayers. Physical Review Letters, 1993, 71, 1923-1926.	7.8	106
99	First-principles study of phase stability of Tiâ€“Al intermetallic compounds. Journal of Materials Research, 1993, 8, 2554-2568.	2.6	105
100	First-principles phase-stability study of fcc alloys in the Ti-Al system. Physical Review B, 1992, 46, 5055-5072.	3.2	122
101	van Schilfgaarde and Newman reply. Physical Review Letters, 1991, 67, 282-282.	7.8	5
102	Spinâ€polarized band structure of magnetically coupled multilayers. Journal of Applied Physics, 1991, 69, 4783-4785.	2.5	111
103	Electronic structure of ideal metal/GaAs contacts. Physical Review Letters, 1990, 65, 2728-2731.	7.8	52
104	Quasichemical approximation in binary alloys. Physical Review B, 1987, 36, 4279-4295.	3.2	130
105	Tight-binding theory and elastic constants. Physical Review B, 1987, 36, 4375-4382.	3.2	15
106	Tightâ€binding theory of force constant models. Applied Physics Letters, 1987, 51, 175-176.	3.3	3
107	Coulomb Energy in Pseudobinary Alloys. Physical Review Letters, 1986, 57, 1149-1152.	7.8	20
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109	Electronic structure of boron. Journal of Physics and Chemistry of Solids, 1985, 46, 1093-1100.	4.0	41