Mark Van Schilfgaarde

List of Publications by Year
in descending order

109 papers	16,589 citations	28272 55 h-index	24978 109 g-index
109 all docs	109 docs citations	109 times ranked	16542 citing authors

#	Article	IF	Citations
1	Ionic transport in hybrid lead iodide perovskite solar cells. Nature Communications, 2015, 6, 7497.	12.8	2,154
2	Atomistic Origins of High-Performance in Hybrid Halide Perovskite Solar Cells. Nano Letters, 2014, 14, 2584-2590.	9.1	2,068
3	Reversible Hydration of CH₃NH₃PbI₃ in Films, Single Crystals, and Solar Cells. Chemistry of Materials, 2015, 27, 3397-3407.	6.7	1,133
4	Relativistic quasiparticle self-consistent electronic structure of hybrid halide perovskite photovoltaic absorbers. Physical Review B, 2014, 89, .	3.2	612
5	Origin of the Invar effect in ironâ€“nickel alloys. Nature, 1999, 400, 46-49.	27.8	487
6	Molecular ferroelectric contributions to anomalous hysteresis in hybrid perovskite solar cells. APL Materials, 2014, 2, .	5.1	481
7	All-Electron Self-ConsistentGWApproximation: Application to Si, MnO, and NiO. Physical Review Letters, 2004, 93, 126406.	7.8	475
8	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
9	Lattice dynamics and vibrational spectra of the orthorhombic, tetragonal, and cubic phases of methylammonium lead iodide. Physical Review B, 2015, 92, .	3.2	452
10	What Is Moving in Hybrid Halide Perovskite Solar Cells?. Accounts of Chemical Research, 2016, 49, 528-535.	15.6	385
11	Experimental and theoretical optical properties of methylammonium lead halide perovskites. Nanoscale, 2016, 8, 6317-6327.	5.6	385
12	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
13	Ferroelectric materials for solar energy conversion: photoferroics revisited. Energy and Environmental Science, 2015, 8, 838-848.	30.8	333
14	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
15	Real-Time Observation of Organic Cation Reorientation in Methylammonium Lead Iodide Perovskites. Journal of Physical Chemistry Letters, 2015, 6, 3663-3669.	4.6	322
16	Indirect to direct bandgap transition in methylammonium lead halide perovskite. Energy and Environmental Science, 2017, 10, 509-515.	30.8	318
17	Band alignment of the hybrid halide perovskites CH₃NH₃PbCl₃, CH₃NH₃PbBr₃and CH₃NH₃PbI₃. Materials Horizons, 2015, 2, 228-231.	12.2	238
18	Effective masses and valence-band splittings in GaN and AlN. Physical Review B, 1997, 56, 7363-7375.	3.2	226

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19	Role of microstructure in the electronâ€“hole interaction of hybrid lead halide perovskites. Nature Photonics, 2015, 9, 695-701.	31.4	226
20	Direct Observation of Dynamic Symmetry Breaking above Room Temperature in Methylammonium Lead Iodide Perovskite. ACS Energy Letters, 2016, 1, 880-887.	17.4	221
21	AbÂInitioPrediction of Conduction Band Spin Splitting in Zinc Blende Semiconductors. Physical Review Letters, 2006, 96, 086405.	7.8	193
22	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
23	Research Update: Relativistic origin of slow electron-hole recombination in hybrid halide perovskite solar cells. APL Materials, 2016, 4, .	5.1	178
24	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
25	Origin of Pronounced Nonlinear Band Gap Behavior in Leadâ€“Tin Hybrid Perovskite Alloys. Chemistry of Materials, 2018, 30, 3920-3928.	6.7	166
26	Models of charge pair generation in organic solar cells. Physical Chemistry Chemical Physics, 2015, 17, 2311-2325.	2.8	158
27	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
28	Adequacy of approximations inGWtheory. Physical Review B, 2006, 74, .	3.2	149
29	Emergent Properties of an Organic Semiconductor Driven by its Molecular Chirality. ACS Nano, 2017, 11, 8329-8338.	14.6	136
30	Quasichemical approximation in binary alloys. Physical Review B, 1987, 36, 4279-4295.	3.2	130
31	First-principles phase-stability study of fcc alloys in the Ti-Al system. Physical Review B, 1992, 46, 5055-5072.	3.2	122
32	Computational Screening of All Stoichiometric Inorganic Materials. CheM, 2016, 1, 617-627.	11.7	115
33	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
34	Spinâ€polarized band structure of magnetically coupled multilayers. Journal of Applied Physics, 1991, 69, 4783-4785.	2.5	111
35	Perspective: Theory and simulation of hybrid halide perovskites. Journal of Chemical Physics, 2017, 146, 220901.	3.0	111
36	Spin lifetimes of electrons injected into GaAs and GaN. Applied Physics Letters, 2003, 83, 1761-1763.	3.3	109

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37	Simplified first principles approach to exchange coupling in magnetic multilayers. Physical Review Letters, 1993, 71, 1923-1926.	7.8	106
38	First-principles study of phase stability of Tiâ€“Al intermetallic compounds. Journal of Materials Research, 1993, 8, 2554-2568.	2.6	105
39	Computational materials design of crystalline solids. Chemical Society Reviews, 2016, 45, 6138-6146.	38.1	105
40	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
41	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
42	Fusion of the LAPW and LMTO methods: The augmented plane wave plus muffin-tin orbital method. Physical Review B, 2010, 81, .	3.2	90
43	Questaal: A package of electronic structure methods based on the linear muffin-tin orbital technique. Computer Physics Communications, 2020, 249, 107065.	7.5	82
44	Ab initiotight-binding LMTO method for nonequilibrium electron transport in nanosystems. Physical Review B, 2005, 71, .	3.2	81
45	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
46	Pressure-Induced Invar Effect in Fe-Ni Alloys. Physical Review Letters, 2001, 86, 4851-4854.	7.8	78
47	Reversal of Spin Polarization inFe/GaAs(001) Driven by Resonant Surface States: First-Principles Calculations. Physical Review Letters, 2007, 99, 196603.	7.8	75
48	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
49	Oscillatory exchange coupling: RKKY or quantum-well mechanism?. Physical Review Letters, 1993, 71, 3870-3873.	7.8	69
50	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
51	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
52	Impact of nonparabolic electronic band structure on the optical and transport properties of photovoltaic materials. Physical Review B, 2019, 99, .	3.2	60
53	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
54	Theory of the multicenter bond. Physical Review B, 1986, 33, 2653-2659.	3.2	58

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55	Direct method for calculating temperature-dependent transport properties. Physical Review B, 2015, 91, .	3.2	57
56	Theoretical study of environmental dependence of oxygen vacancy formation in CeO2. Applied Physics Letters, 2005, 87, 141917.	3.3	56
57	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
58	First-principles treatment of Mott insulators: linearized QSGW+DMFT approach. Npj Quantum Materials, 2016, 1, .	5.2	54
59	Bandstructure effect on high-field transport in GaN and GaAlN. Applied Physics Letters, 1997, 71, 1999-2001.	3.3	53
60	Electronic structure of ideal metal/GaAs contacts. Physical Review Letters, 1990, 65, 2728-2731.	7.8	52
61	Dynamic symmetry breaking and spin splitting in metal halide perovskites. Physical Review B, 2018, 98, .	3.2	52
62	Theory of Oscillatory Exchange Coupling in Fe/(V,Cr) and Fe/(Cr,Mn). Physical Review Letters, 1995, 74, 4063-4066.	7.8	50
63	InTlSb: An infrared detector material?. Applied Physics Letters, 1993, 62, 1857-1859.	3.3	47
64	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
65	Band-filling effect on magnetic anisotropy using a Green's function method. Physical Review B, 2015, 92, .	3.2	42
66	Electronic structure of boron. Journal of Physics and Chemistry of Solids, 1985, 46, 1093-1100.	4.0	41
67	Self-energies in itinerant magnets: A focus on Fe and Ni. Physical Review B, 2017, 95, .	3.2	39
68	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
69	Anisotropic Plasmonic CuS Nanocrystals as a Natural Electronic Material with Hyperbolic Optical Dispersion. ACS Nano, 2019, 13, 6550-6560.	14.6	30
70	Electronic properties of alkali-metal loaded zeolites: Supercrystal Mott insulators. Physical Review B, 2004, 69, .	3.2	27
71	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
72	Quasiparticle self-consistentGWmethod: a short summary. Journal of Physics Condensed Matter, 2007, 19, 365236.	1.8	24

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73	Spin filtering with EuO: Insight from the complex band structure. Physical Review B, 2012, 85, .	3.2	24
74	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
75	Coulomb Energy in Pseudobinary Alloys. Physical Review Letters, 1986, 57, 1149-1152.	7.8	20
76	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
77	Thin film tandem photovoltaic cell from II-IV-V chalcopyrites. Applied Physics Letters, 2010, 96, 143503.	3.3	18
78	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
79	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></mml:math> including electron-hole interaction effects. Physical Review B, 2021, 104, .	3.2	18
80	Electronic structure of chromium trihalides beyond density functional theory. Physical Review B, 2021, 104, .	3.2	18
81	Tight-binding theory and elastic constants. Physical Review B, 1987, 36, 4375-4382.	3.2	15
82	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
83	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
84	GW quasiparticle band structure of CaB6. Journal of Physics and Chemistry of Solids, 2002, 63, 1595-1597.	4.0	13
85	Criteria for improving the properties of ZnGeAs₂ solar cells. Progress in Photovoltaics: Research and Applications, 2013, 21, 906-917.	8.1	13
86	Importance of charge self-consistency in first-principles description of strongly correlated systems. Npj Computational Materials, 2021, 7, .	8.7	13
87	Low-energy coherent Stoner-like excitations inCaFe2As2. Physical Review B, 2011, 83, .	3.2	12
88	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
89	Spin excitations in K<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 />	3.2	11
90	Effect of correlations on electronic structure and transport across (001) Fe/MgO/Fe junctions. Physical Review B, 2012, 85, .	3.2	11

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91	The magnetic, electrical and structural properties of copper-permalloy alloys. Journal of Magnetism and Magnetic Materials, 2017, 442, 45-52.	2.3	11
92	Metal-Insulator Transition in Copper Oxides Induced by Apex Displacements. Physical Review X, 2018, 8, .	8.9	11
93	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
94	Electronic Origin of Tc in Bulk and Monolayer FeSe. Symmetry, 2021, 13, 169.	2.2	9
95	Ultrafast Carrier and Lattice Dynamics in Plasmonic Nanocrystalline Copper Sulfide Films. Laser and Photonics Reviews, 2021, 15, 2000346.	8.7	9
96	Role of the lattice in the light-induced insulator-to-metal transition in vanadium dioxide. Physical Review Research, 2020, 2, .	3.6	9
97	Supercurrent decay in ballistic magnetic Josephson junctions. Npj Computational Materials, 2022, 8, .	8.7	9
98	Direct gap in ordered silicon carbon alloys. Applied Physics Letters, 1999, 75, 3153-3155.	3.3	7
99	Breakdown of a gold nanowire between electrodes. Nanotechnology, 2007, 18, 424002.	2.6	7
100	Magnetic properties of chromium-doped Ni80Fe20 thin films. Journal of Magnetism and Magnetic Materials, 2018, 460, 193-202.	2.3	7
101	van Schilfgaarde and Newman reply. Physical Review Letters, 1991, 67, 282-282.	7.8	5
102	Electronic Structure Correspondence of Singlet-Triplet Scale Separation in Strained Sr2RuO4. Applied Sciences (Switzerland), 2021, 11, 508.	2.5	4
103	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
104	Tightâ€binding theory of force constant models. Applied Physics Letters, 1987, 51, 175-176.	3.3	3
105	Electronic and optical properties of crystalline nitrogen versus black phosphorus: A comparative first-principles study. Physical Review B, 2022, 105, .	3.2	3
106	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:n self-energy and its application to defect calculations. Physical Review B, 2022, 105, .	3.2	2
107	Theoretical and Experimental Study of Barium Zinc-Cadmium Tantalate-based Microwave Dielectrics. Materials Research Society Symposia Proceedings, 2003, 783, 471.	0.1	1
108	A First Principles Alloy Scattering Approach for Monte Carlo Hole Mobility Calculations. Journal of Computational Electronics, 2004, 3, 351-354.	2.5	1

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109	Doping-induced metallicity and coexistence of magnetic subsystems in K2Fe4+xSe5. Solid State Communications, 2012, 152, 1846-1849.	1.9	1