Andre Schleife

List of Publications by Year
in descending order

90 papers	3,608 citations	109321 35 h-index	133252 59 g-index
90 all docs	90 docs citations	90 times ranked	4135 citing authors

#	Article	IF	Citations
1	First-principles study of ground- and excited-state properties ofMgO,ZnO, andCdOpolymorphs. Physical Review B, 2006, 73, .	3.2	361
2	Branch-point energies and band discontinuities of III-nitrides and III-/II-oxides from quasiparticle band-structure calculations. Applied Physics Letters, 2009, 94, .	3.3	177
3	First-Principles Optical Spectra for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>F</mml:mi></mml:math>Centers in MgO. Physical Review Letters, 2012, 108, 126404.	7.8	157
4	Tin dioxide from first principles: Quasiparticle electronic states and optical properties. Physical Review B, 2011, 83, .	3.2	145
5	Optical and energy-loss spectra of MgO, ZnO, and CdO fromab initiomany-body calculations. Physical Review B, 2009, 80, .	3.2	142
6	Valence-band electronic structure of CdO, ZnO, and MgO from x-ray photoemission spectroscopy and quasi-particle-corrected density-functional theory calculations. Physical Review B, 2009, 79, .	3.2	124
7	Accurate atomistic first-principles calculations of electronic stopping. Physical Review B, 2015, 91, .	3.2	121
8	Efficient<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="script">O</mml:mi><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:msup><mml:mi>N</mml:mi><mml:mn>2</mml:m to solve the Bethe-Salpeter equation for excitonic bound states. Physical Review B, 2008, 78, .	3.2	117
9	Ambipolar doping in SnO. Applied Physics Letters, 2013, 103, .	3.3	94
10	Plane-wave pseudopotential implementation of explicit integrators for time-dependent Kohn-Sham equations in large-scale simulations. Journal of Chemical Physics, 2012, 137, 22A546.	3.0	80
11	Deep Learning Enabled Strain Mapping of Single-Atom Defects in Two-Dimensional Transition Metal Dichalcogenides with Sub-Picometer Precision. Nano Letters, 2020, 20, 3369-3377.	9.1	78
12	Observation of quantized subband states and evidence for surface electron accumulation in CdO from angle-resolved photoemission spectroscopy. Physical Review B, 2008, 78, .	3.2	75
13	Quantum dot surface engineering: Toward inert fluorophores with compact size and bright, stable emission. Coordination Chemistry Reviews, 2016, 320-321, 216-237.	18.8	74
14	Role of Surface Termination on Hot Electron Relaxation in Silicon Quantum Dots: A First-Principles Dynamics Simulation Study. Nano Letters, 2015, 15, 6429-6433.	9.1	73
15	Band structure of ZnO from resonant x-ray emission spectroscopy. Physical Review B, 2008, 78, .	3.2	70
16	Bandâ€structure and opticalâ€transition parameters of wurtzite MgO, ZnO, and CdO from quasiparticle calculations. Physica Status Solidi (B): Basic Research, 2009, 246, 2150-2153.	1.5	68
17	Electron Elevator: Excitations across the Band Gap via a Dynamical Gap State. Physical Review Letters, 2016, 116, 043201.	7.8	68
18	Optical-helicity-driven magnetization dynamics in metallic ferromagnets. Nature Communications, 2017, 8, 15085.	12.8	68

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19	Band discontinuities at Si-TCO interfaces from quasiparticle calculations: Comparison of two alignment approaches. Physical Review B, 2012, 85, .	3.2	62
20	Optical Absorption in Degenerately Doped Semiconductors: Mott Transition or Mahan Excitons?. Physical Review Letters, 2011, 107, 236405.	7.8	61
21	Electronic and optical properties of Mg_xZn_{1â^'x}O and Cd_xZn_{1â^'x}O fromab initiocalculations. New Journal of Physics, 2011, 13, 085012.	2.9	60
22	Metallic antiferromagnets. Journal of Applied Physics, 2020, 128, .	2.5	57
23	Strain influence on valence-band ordering and excitons in ZnO: Anab initiostudy. Applied Physics Letters, 2007, 91, 241915.	3.3	55
24	The 2021 ultrafast spectroscopic probes of condensed matter roadmap. Journal of Physics Condensed Matter, 2021, 33, 353001.	1.8	55
25	Ab initiodescription of heterostructural alloys: Thermodynamic and structural properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Mg</mml:mtext></mml:mrow><mml:mi>x</mml:mi></mml:msub xmlns:mml="http://www.w3.org/1998/Math/MathM. Physical Review B, 2010, 81, .	3.2	49
26	Band lineup between silicon and transparent conducting oxides. Applied Physics Letters, 2010, 97, .	3.3	48
27	Interplay of excitonic effects and van Hove singularities in optical spectra: CaO and AlN polymorphs. Physical Review B, 2011, 84, .	3.2	46
28	Structural, electrical, and optical properties of hydrogen-doped ZnO films. Physical Review B, 2012, 86, .	3.2	43
29	Massively parallel first-principles simulation of electron dynamics in materials. Journal of Parallel and Distributed Computing, 2017, 106, 205-214.	4.1	42
30	Quantum Dynamics Simulation of Electrons in Materials on High-Performance Computers. Computing in Science and Engineering, 2014, 16, 54-60.	1.2	41
31	Tuning Electronic Structure in Layered Hybrid Perovskites with Organic Spacer Substitution. Nano Letters, 2019, 19, 8732-8740.	9.1	41
32	Photoemission spectra and effective masses of nâ€•and pâ€type oxide semiconductors from first principles: ZnO, CdO, SnO₂, MnO, and NiO. Physica Status Solidi (A) Applications and Materials Science, 2014, 211, 74-81.	1.8	40
33	Betheâ€“Salpeter calculation of optical-absorption spectra of In₂O₃and Ga₂O₃. Semiconductor Science and Technology, 2015, 30, 024010.	2.0	38
34	Solid-State Divalent Ion Conduction in ZnPS₃. Chemistry of Materials, 2019, 31, 3652-3661.	6.7	37
35	Multiscale simulations of electron and ion dynamics in self-irradiated silicon. Physical Review B, 2020, 102, .	3.2	37
36	Electronic structure of single-crystal rocksalt CdO studied by soft x-ray spectroscopies andab initiocalculations. Physical Review B, 2008, 77, .	3.2	35

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37	Origin of resolution enhancement by co-doping of scintillators: Insight from electronic structure calculations. Applied Physics Letters, 2014, 104, .	3.3	34
38	Quasiparticle spectra, absorption spectra, and excitonic properties of NaI and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>SrI</mml:mi></mml:mrow><mml:mn>2</mml:mn>2</mml:msub></mml:math> from many-body perturbation theory. Physical Review B, 2014, 89, .	3.2	32
39	Carrier-Specific Femtosecond XUV Transient Absorption of PbI₂ Reveals Ultrafast Nonradiative Recombination. Journal of Physical Chemistry C, 2017, 121, 27886-27893.	3.1	30
40	Ab initio description of quasiparticle band structures and optical near-edge absorption of transparent conducting oxides. Journal of Materials Research, 2012, 27, 2180-2189.	2.6	29
41	Optical determination of crystal phase in semiconductor nanocrystals. Nature Communications, 2017, 8, 14849.	12.8	29
42	Valence-band splittings in cubic and hexagonal AlN, GaN, and InN. Applied Physics Letters, 2010, 97, .	3.3	28
43	First-principles study of codoping in lanthanum bromide. Physical Review B, 2015, 91, .	3.2	27
44	Ab-Initio Studies of Electronic and Spectroscopic Properties of MgO, ZnO and CdO. Journal of the Korean Physical Society, 2008, 53, 2811-2815.	0.7	26
45	Influence of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Ï€</mml:mi></mml:math> -conjugated cations and halogen substitution on the optoelectronic and excitonic properties of layered hybrid perovskites. Physical Review Materials, 2018, 2, .	2.4	24
46	Databaseâ€Driven Materials Selection for Semiconductor Heterojunction Design. Advanced Theory and Simulations, 2018, 1, 1800075.	2.8	23
47	Anomalous Stopping and Charge Transfer in Proton-Irradiated Graphene. Nano Letters, 2021, 21, 4816-4822.	9.1	23
48	Distribution of cations in wurtzitic In<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>Ga<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>N and In<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:mat. Physical Revie.	3.2	22
49	Ultrafast dynamics of hot charge carriers in an oxide semiconductor probed by femtosecond spectroscopic ellipsometry. New Journal of Physics, 2020, 22, 083066.	2.9	21
50	Optical properties of In₂O₃ from experiment and first-principles theory: influence of lattice screening. New Journal of Physics, 2018, 20, 053016.	2.9	20
51	Pre-equilibrium stopping and charge capture in proton-irradiated aluminum sheets. Physical Review B, 2020, 102, .	3.2	20
52	Clustering of N impurities in ZnO. Applied Physics Letters, 2012, 100, 022107.	3.3	18
53	Pushing the frontiers of modeling excited electronic states and dynamics to accelerate materials engineering and design. Computational Materials Science, 2019, 160, 207-216.	3.0	18
54	Real-Time Exciton Dynamics with Time-Dependent Density-Functional Theory. Physical Review Letters, 2021, 127, 077401.	7.8	17

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55	Carrier-Specific Hot Phonon Bottleneck in CH₃NH₃PbI₃ Revealed by Femtosecond XUV Absorption. Journal of the American Chemical Society, 2021, 143, 20176-20182.	13.7	16
56	Electronic stopping and proton dynamics in InP, GaP, and In0.5Ga0.5P from first principles. European Physical Journal B, 2018, 91, 1.	1.5	15
57	Hot-Electron-Mediated Ion Diffusion in Semiconductors for Ion-Beam Nanostructuring. Nano Letters, 2019, 19, 3939-3947.	9.1	15
58	Electron cascades and secondary electron emission in graphene under energetic ion irradiation. Physical Review B, 2021, 103, .	3.2	15
59	Ab initiocalculation of optical properties with excitonic effects in wurtzite InxGa1â^'xN and InxAl1â^'xN alloys. Physical Review B, 2013, 87, .	3.2	14
60	Enhanced Optical Absorption Due to Symmetry Breaking in TiO_{2(1â€“x)}S_{2x} Alloys. Journal of Physical Chemistry C, 2013, 117, 4189-4193.	3.1	13
61	Auger recombination in sodium-iodide scintillators from first principles. Applied Physics Letters, 2015, 106, .	3.3	11
62	Strain and screening: Optical properties of a small-diameter carbon nanotube from first principles. Physical Review B, 2019, 99, .	3.2	10
63	Nonequilibrium BN-ZnO: Optical properties and excitonic effects from first principles. Physical Review B, 2018, 97, .	3.2	9
64	Magneto-optic response of the metallic antiferromagnet <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Fe</mml:mi><mml:mn>2</mml:mn></mml:r to ultrafast temperature excursions. Physical Review Materials, 2019, 3, .	3.1	9
65	Revealing the Sequence-Structureâ€“Electronic Property Relation of Self-Assembling Ï€-Conjugated Oligopeptides by Molecular and Quantum Mechanical Modeling. Langmuir, 2019, 35, 15221-15231.	3.5	8
66	Transient birefringence and dichroism in ZnO studied with fs-time-resolved spectroscopic ellipsometry. Physical Review Research, 2021, 3, .	3.6	8
67	Computational discovery of high charge mobility self-assembling Ï€-conjugated peptides. Molecular Systems Design and Engineering, 2022, 7, 447-459.	3.4	8
68	Voltage-induced switching of an antiferromagnetically ordered topological Dirac semimetal. Physical Review B, 2018, 97, .	3.2	7
69	Free-electron effects on the optical absorption of the hybrid perovskite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>CH</mml:mi><mml:mn>3</mml:mn></mml: from first principles. Physical Review B, 2019, 100, .	3.2	7
70	New Family of Anisotropic Zinc-Based Semiconductors in a Shallow Energy Landscape. Chemistry of Materials, 2020, 32, 326-332.	6.7	7
71	Magnetocrystalline anisotropy of the easy-plane metallic antiferromagnet <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">F</mml:mi><mml:msub><mml:mi mathvariant="normal">e</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi>As</mml:mi></mml:mrow></mml:math>. Physical Review B, 2020, 102, .	3.2	7
72	Excitons in scintillator materials: Optical properties and electron-energy loss spectra of NaI, LaBr₃, BaI₂, and SrI₂. Journal of Materials Research, 2017, 32, 56-63.	2.6	6

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73	Structural, Electronic, and Optical Properties of K2Sn3O7 with an Offset Hollandite Structure. Inorganic Chemistry, 2017, 56, 2914-2918.	4.0	5
74	Strongly two-dimensional exchange interactions in the in-plane metallic antiferromagnet <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Fe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> probed by inelastic neutron scattering. Physical Review Materials, 2020, 4, .	2.4	5
75	Low-energy electronic structure of perovskite and Ruddlesden-Popper semiconductors in the Ba-Zr-S system probed by bond-selective polarized x-ray absorption spectroscopy, infrared reflectivity, and Raman scattering. Physical Review B, 2022, 105, .	3.2	5
76	Impact of degeneraten-doping on the optical absorption edge in transparent conducting cadmium oxide. , 2013, , .		4
77	Solving the Bethe-Salpeter equation on massively parallel architectures. Computer Physics Communications, 2021, 267, 108081.	7.5	4
78	In-plane hexagonal antiferromagnet in the Cu-Mn-As system <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Cu</mml:mi><mml:mrow><mml:mn>0.82</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Physical Review Materials, 2019, 3, .	2.4	4
79	Conductivity and transparency of TiO2from first principles. , 2013, , .		2
80	Optimization of anisotropic photonic density of states for Raman cooling of solids. Physical Review A, 2018, 97, .	2.5	2
81	Probing the Strain Fields of Single-Atom Defects in 2D materials with Sub-Picometer Precision. Microscopy and Microanalysis, 2021, 27, 1944-1944.	0.4	2
82	Computational Curriculum for MatSE Undergraduates. , 0, , .		2
83	Morphology and Growth Habit of the New Flux-Grown Layered Semiconductor KBiS₂ Revealed by Diffraction Contrast Tomography. Crystal Growth and Design, 2022, 22, 3228-3234.	3.0	2
84	Delocalization of dark and bright excitons in flat-band materials and the optical properties of V2O5. Npj Computational Materials, 2022, 8, .	8.7	2
85	Polar magneto-optical Kerr effect in antiferromagnetic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>M</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">As</mml:mi><mml:mo>Â</mml:mo><mml:mrow><mml:mo>(</mml:mo><mml:mi>M</mml:mi><mml:mo>=	3.2	2
86	Novel diffusion mechanism in the presence of excited electrons?. Materials Today, 2018, 21, 925-927.	14.2	1
87	In-plane magnetic structure and exchange interactions in the high-temperature antiferromagnet Cr2Al. Physical Review Materials, 2021, 5, .	2.4	1
88	Detecting Vacancy-Induced Strain Field Oscillations via Deep Learning. Microscopy and Microanalysis, 2020, 26, 14-16.	0.4	0
89	Understanding Carrier Specific Dynamics in CH3NH3PbBr3 by Femtosecond Tabletop Extreme Ultraviolet Spectroscopy. , 2020, , .		0
90	Structure and Magnetic Properties of Ni₄V₃O₁₀, an Antiferromagnet with Three Types of Vanadiumâ€“Oxygen Polyhedra. Chemistry of Materials, 2022, 34, 4721-4731.	6.7	0