Matthieu J Verstraete

List of Publications by Year
in descending order

104	11,831	159585 30	30922 102
papers	citations	h-index	g-index

106	106	106	9909
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	First-principles computation of material properties: the ABINIT software project. Computational Materials Science, 2002, 25, 478-492.	3.0	2,789
2	ABINIT: First-principles approach to material and nanosystem properties. Computer Physics Communications, 2009, 180, 2582-2615.	7.5	2,297
3	A brief introduction to the ABINIT software package. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.8	1,101
4	The PseudoDojo: Training and grading a 85 element optimized norm-conserving pseudopotential table. Computer Physics Communications, 2018, 226, 39-54.	7.5	1,001
5	BoltzTraP2, a program for interpolating band structures and calculating semi-classical transport coefficients. Computer Physics Communications, 2018, 231, 140-145.	7.5	730
6	Recent developments in the ABINIT software package. Computer Physics Communications, 2016, 205, 106-131.	7.5	662
7	Real-space grids and the Octopus code as tools for the development of new simulation approaches for electronic systems. Physical Chemistry Chemical Physics, 2015, 17, 31371-31396.	2.8	376
8	The Abinitproject: Impact, environment and recent developments. Computer Physics Communications, 2020, 248, 107042.	7.5	369
9	The high conductivity of iron and thermal evolution of the Earthâ€™s core. Physics of the Earth and Planetary Interiors, 2013, 224, 88-103.	1.9	251
10	ABINIT: Overview and focus on selected capabilities. Journal of Chemical Physics, 2020, 152, 124102.	3.0	179
11	Temperature dependence of the electronic structure of semiconductors and insulators. Journal of Chemical Physics, 2015, 143, 102813.	3.0	139
12	Thermal conductivity in PbTe from first principles. Physical Review B, 2015, 91, .	3.2	98
13	Electron-Beam Manipulation of Silicon Dopants in Graphene. Nano Letters, 2018, 18, 5319-5323.	9.1	98
14	TB2J: A python package for computing magnetic interaction parameters. Computer Physics Communications, 2021, 264, 107938.	7.5	92
15	Two-Step Phase Transition in SnSe and the Origins of its High Power Factor from First Principles. Physical Review Letters, 2016, 117, 276601.	7.8	91
16	First Principles Explanation of the Positive Seebeck Coefficient of Lithium. Physical Review Letters, 2014, 112, 196603.	7.8	68
17	Density functional perturbation theory with spin-orbit coupling: Phonon band structure of lead. Physical Review B, 2008, 78, .	3.2	66
18	First-principles calculation of the electronic, dielectric, and dynamical properties ofCaF2. Physical Review B, 2003, 68, .	3.2	62

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19	Density functional theory beyond the linear regime: Validating an adiabatic local density approximation. Physical Review A, 2011, 83, .	2.5	61
20	Electron-Phonon beyond FrÃ¶hlich: Dynamical Quadrupoles in Polar and Covalent Solids. Physical Review Letters, 2020, 125, 136601.	7.8	60
21	Thermopower in oxide heterostructures: The importance of being multiple-band conductors. Physical Review B, 2012, 86, .	3.2	48
22	Phonon-limited electron mobility in Si, GaAs, and GaP with exact treatment of dynamical quadrupoles. Physical Review B, 2020, 102, .	3.2	47
23	Electronic properties of the Mg2Si thermoelectric material investigated by linear-response density-functional theory. Computational Materials Science, 2011, 50, 847-851.	3.0	46
24	Doping-induced dimensional crossover and thermopower burst in Nb-doped SrTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>superlattices. Physical Review B, 2013, 88, .	3.2	40
25	High Temperature Ferromagnetism in a GdAg₂ Monolayer. Nano Letters, 2016, 16, 4230-4235.	9.1	40
26	The psml format and library for norm-conserving pseudopotential data curation and interoperability. Computer Physics Communications, 2018, 227, 51-71.	7.5	38
27	Are Hydrogen-Bonded Charge Transfer Crystals Room Temperature Ferroelectrics?. Physical Review Letters, 2014, 113, 237602.	7.8	35
28	Aluminum Conducts Better than Copper at the Atomic Scale: A First-Principles Study of Metallic Atomic Wires. ACS Nano, 2012, 6, 10449-10455.	14.6	34
29	Origin of the counterintuitive dynamic charge in the transition metal dichalcogenides. Physical Review B, 2017, 95, .	3.2	34
30	Smearing scheme for finite-temperature electronic-structure calculations. Physical Review B, 2001, 65, .	3.2	32
31	Thermodynamic, thermoelectric, and magnetic properties of FeSb<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>: A combined first-principles and experimental study. Physical Review B, 2011, 84, .	3.2	30
32	Cumulant expansion for phonon contributions to the electron spectral function. Physical Review B, 2014, 90, .	3.2	30
33	The physics of single-side fluorination of graphene: DFT and DFTÂ+ U studies. Carbon, 2019, 144, 615-627.	10.3	30
34	Effect of hydrostatic pressure on the thermoelectric properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="bold">Bi</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">Te</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2014, 90, .	3.2	29
35	First-principles study of the lattice dynamical properties of strontium ruthenate. Journal of Physics Condensed Matter, 2014, 26, 035401.	1.8	29
36	Ab initiostudy ofMoS2nanotube bundles. Physical Review B, 2003, 68, .	3.2	27

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37	First-Principles Study of the Thermoelectric Properties of SrRuO3. Journal of Physical Chemistry C, 2016, 120, 9112-9121.	3.1	27
38	Spin States Protected from Intrinsic Electronâ€“Phonon Coupling Reaching 100 ns Lifetime at Room Temperature in MoSe2. Nano Letters, 2019, 19, 4083-4090.	9.1	27
39	Why is iridium the best substrate for single crystal diamond growth?. Applied Physics Letters, 2005, 86, 191917.	3.3	26
40	Ab initiocalculation of spin-dependent electronâ€“phonon coupling in iron and cobalt. Journal of Physics Condensed Matter, 2013, 25, 136001.	1.8	26
41	Vibrational and dielectric properties of the bulk transition metal dichalcogenides. Physical Review Materials, 2018, 2, .	2.4	25
42	Nonmonotonic anisotropy in charge conduction induced by antiferrodistortive transition in metallic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></m Physical Review B, 2016, 94, .	3.2	23
43	Rare-Earth Surface Alloying: A New Phase for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>GdAu</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. PhysicalReviewLetters, 2015, 115, 016101.	7.8	22
44	LaAu<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>and CeAu<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>surface intermetallic compounds grown by high-temperature deposition on Au(111). Physical Review B, 2013, 88, .	3.2	21
45	Electronic and Thermoelectric Properties of Transition-Metal Dichalcogenides. Journal of Physical Chemistry C, 2021, 125, 27084-27097.	3.1	21
46	Phonon band structure and electron-phonon interactions in metallic nanowires. Physical Review B, 2006, 74, .	3.2	20
47	Phases of Polonium via Density Functional Theory. Physical Review Letters, 2010, 104, 035501.	7.8	20
48	Low-Energy Phases of Bi Monolayer Predicted by Structure Search in Two Dimensions. Journal of Physical Chemistry Letters, 2019, 10, 7324-7332.	4.6	18
49	Anomalous ESR behavior of carbon nanofilaments grown from palladium seeds. Carbon, 2004, 42, 1049-1052.	10.3	17
50	Electron mobility in monolayer WS2 encapsulated in hexagonal boron-nitride. Applied Physics Letters, 2021, 118, .	3.3	17
51	Role of Dynamical Instability in theAbÂInitioPhase Diagram of Calcium. Physical Review Letters, 2013, 111, 025503.	7.8	16
52	Quantitative Agreement between Electron-Optical Phase Images of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>WSe</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Simulations Based on Electrostatic Potentials that Include Bonding Effects. Physical Review Letters, 2017, 118, 086101.	7.8	15
53	From one to three, exploring the rungs of Jacobâ€™s ladder in magnetic alloys. European Physical Journal B, 2018, 91, 1.	1.5	15
54	Strain-induced effects in the electronic and spin properties of a monolayer of ferromagnetic GdAg₂. Nanoscale, 2016, 8, 19148-19153.	5.6	13

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55	Thermoelectric properties of elemental metals from first-principles electron-phonon coupling. Physical Review B, 2020, 102, .	3.2	13
56	Phonon-Assisted Luminescence in Defect Centers from Many-Body Perturbation Theory. Physical Review Letters, 2022, 128, 167401.	7.8	13
57	First-principles study of transport properties in Os and OsSi. Physical Review B, 2013, 87, .	3.2	12
58	Spectroscopic properties of few-layer tin chalcogenides. JPhys Materials, 2019, 2, 044005.	4.2	12
59	Remote free-carrier screening to boost the mobility of FrÃ¶hlich-limited two-dimensional semiconductors. Physical Review Materials, 2021, 5, .	2.4	12
60	Unraveling Heat Transport and Dissipation in Suspended MoSe₂ from Bulk to Monolayer. Advanced Materials, 2022, 34, e2108352.	21.0	12
61	Functionality in single-molecule devices: Model calculations and applications of the inelastic electron tunneling signal in molecular junctions. Journal of Chemical Physics, 2012, 136, 064708.	3.0	11
62	Computational Benchmarking for Ultrafast Electron Dynamics: Wave Function Methods vs Density Functional Theory. Journal of Chemical Theory and Computation, 2015, 11, 2221-2233.	5.3	11
63	Conflicting evidence for ferroelectricity. Nature, 2017, 547, E9-E10.	27.8	10
64	Hybrid quantum anomalous Hall effect at graphene-oxide interfaces. Physical Review B, 2018, 98, .	3.2	10
65	Vibrational and dielectric properties of monolayer transition metal dichalcogenides. Physical Review Materials, 2019, 3, .	2.4	10
66	Sharing electronic structure and crystallographic data with ETSF_IO. Computer Physics Communications, 2008, 179, 748-758.	7.5	9
67	Thermoelectric properties of the unfilled skutterudite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>FeSb</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> first principles and Seebeck local probes. Physical Review B, 2015, 92, .	3.2	9
68	First-principles study of spin spirals in the multiferroic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">BiFeO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2021, 103, .	3.2	9
69	Structural and electronic properties ofAgâ^Pdsuperlattices. Physical Review B, 2004, 70, .	3.2	8
70	Density functional perturbation theory within noncollinear magnetism. Physical Review B, 2019, 99, .	3.2	8
71	Optical Signatures of Defect Centers in Transition Metal Dichalcogenide Monolayers. Advanced Quantum Technologies, 2021, 4, 2000118.	3.9	8
72	Exploring the elastic and electronic properties of chromium molybdenum diboride alloys. Journal of Alloys and Compounds, 2021, 866, 158885.	5.5	8

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73	FrÃ¶hlich polaron effective mass and localization length in cubic materials: Degenerate and anisotropic electronic bands. Physical Review B, 2021, 104, .	3.2	8
74	Specification of an extensible and portable file format for electronic structure and crystallographic data. Computational Materials Science, 2008, 43, 1056-1065.	3.0	7
75	First-principles conductance of nanoscale junctions from the polarizability of finite systems. Journal of Chemical Physics, 2009, 130, 124715.	3.0	7
76	Heat Capacity and Anisotropic Thermal Conductivity in Cr₂AlC Single Crystals at High Temperature. Journal of Physical Chemistry C, 2020, 124, 24017-24028.	3.1	7
77	Spontaneous interlayer compression in commensurately stacked van der Waals heterostructures. Physical Review B, 2021, 103, .	3.2	7
78	Ab initio calculation of the thermal conductivity of indium antimonide. Semiconductor Science and Technology, 2014, 29, 124002.	2.0	6
79	Modeling the dissociation and ionization of a sputtered organic molecule. Applied Surface Science, 2006, 252, 6459-6462.	6.1	5
80	Demixing processes in AgPd superlattices. Journal of Physics Condensed Matter, 2009, 21, 315002.	1.8	5
81	Quasi-One-Dimensional Metal-Insulator Transitions in Compound Semiconductor Surfaces. Physical Review Letters, 2016, 117, 116101.	7.8	5
82	Competition of lattice and spin excitations in the temperature dependence of spin-wave properties. Physical Review B, 2018, 97, .	3.2	5
83	Magnetic instabilities in doped <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> full-Heusler thermoelectric compounds. Physical Review B, 2019, 100, .	3.2	5
84	Bulk electronic structure of lanthanum hexaboride (<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 312 Td (xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>La</mml:mi><mml:mn>1</mml:mn></mml:msub><mml:msub><mml:mi>B</mml:mi><mml:mn>6</mml:mn></mml:msub></mml:mrow></mml:math>) hard x-ray angle-resolved photoelectron spectroscopy. Physical Review Materials, 2021, 5, .	2.4	5
85	Ab-initio density functional study of defect-free and defective CdO. Physica Status Solidi C: Current Topics in Solid State Physics, 2005, 2, 3548-3551.	0.8	4
86	Zhao etÂal. Reply. Physical Review Letters, 2017, 118, 239602.	7.8	4
87	Lattice dynamics and phase stability of rhombohedral antimony under high pressure. Physical Review B, 2019, 100, .	3.2	4
88	Direct time-domain determination of electron-phonon coupling strengths in chromium. Physical Review B, 2020, 102, .	3.2	4
89	Spectroscopic signatures of nonpolarons: the case of diamond. Physical Chemistry Chemical Physics, 2022, 24, 12580-12591.	2.8	4
90	Three-dimensional ab initio description of vibration-assisted electron knock-on displacements in graphene. Physical Review B, 2022, 105, .	3.2	4

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91	Metals at finite temperature: a modified smearing scheme. Computational Materials Science, 2004, 30, 27-33.	3.0	3
92	Electronic structure of Agâ€“Pd heterostructures. Computational Materials Science, 2004, 30, 34-43.	3.0	3
93	Assessing Nickel Titanium Binary Systems Using Structural Search Methods and Ab Initio Calculations. Journal of Physical Chemistry C, 2021, 125, 1578-1591.	3.1	3
94	Catalyst consumption during growth of carbon nanofilaments on Pd seeds. Applied Physics Letters, 2004, 85, 5376-5378.	3.3	2
95	Gate Control of Spin-Layer-Locking FETs and Application to Monolayer LuIO. Nano Letters, 2021, 21, 7631-7636.	9.1	2
96	Surface Phonons: Theoretical Methods and Results. Springer Handbooks, 2020, , 737-782.	0.6	2
97	Unraveling Heat Transport and Dissipation in Suspended MoSe₂ from Bulk to Monolayer (Adv. Mater. 10/2022). Advanced Materials, 2022, 34, .	21.0	2
98	Atomic structure of theTeâˆ•Si(100)â€(2Ã—1)surface. Physical Review B, 2005, 72, .	3.2	1
99	First-principles computation of the electronic and dynamical properties of solids and nanostructures with ABINIT (abstract only). Journal of Physics Condensed Matter, 2008, 20, 064212.	1.8	1
100	Implementation of density-functional perturbation theory within ABINIT: Projector augmented-waves and spin-orbit. AIP Conference Proceedings, 2012, , .	0.4	1
101	Interference effects in one-dimensional moirÃ© crystals. Carbon, 2022, 186, 416-422.	10.3	1
102	A theoretical approach to ironâ€based superconductors. Annalen Der Physik, 2011, 523, 580-581.	2.4	0
103	(Invited) Ab Initio Exciton and Phonon Dynamics in Transition Metal Dichalcogenides. ECS Meeting Abstracts, 2021, MA2021-01, 598-598.	0.0	0
104	(Invited) Ab Initio Exciton and Phonon Dynamics in Transition Metal Dichalcogenides. ECS Meeting Abstracts, 2020, MA2020-01, 749-749.	0.0	0