Matthieu J Verstraete

List of Publications by Year
in descending order

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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	Interference effects in one-dimensional moirÃ© crystals. Carbon, 2022, 186, 416-422.	10.3	1
2	Unraveling Heat Transport and Dissipation in Suspended MoSe₂ from Bulk to Monolayer. Advanced Materials, 2022, 34, e2108352.	21.0	12
3	Unraveling Heat Transport and Dissipation in Suspended MoSe₂ from Bulk to Monolayer (Adv. Mater. 10/2022). Advanced Materials, 2022, 34, .	21.0	2
4	Phonon-Assisted Luminescence in Defect Centers from Many-Body Perturbation Theory. Physical Review Letters, 2022, 128, 167401.	7.8	13
5	Spectroscopic signatures of nonpolarons: the case of diamond. Physical Chemistry Chemical Physics, 2022, 24, 12580-12591.	2.8	4
6	Three-dimensional ab initio description of vibration-assisted electron knock-on displacements in graphene. Physical Review B, 2022, 105, .	3.2	4
7	Optical Signatures of Defect Centers in Transition Metal Dichalcogenide Monolayers. Advanced Quantum Technologies, 2021, 4, 2000118.	3.9	8
8	Remote free-carrier screening to boost the mobility of FrÃ¶hlich-limited two-dimensional semiconductors. Physical Review Materials, 2021, 5, .	2.4	12
9	Electron mobility in monolayer WS2 encapsulated in hexagonal boron-nitride. Applied Physics Letters, 2021, 118, .	3.3	17
10	Bulk electronic structure of lanthanum hexaboride (<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 392 Td (xmlns:mml="http://www. hard x-ray angle-resolved photoelectron spectroscopy. Physical Review Materials, 2021, 5, .	2.4	5
11	(Invited) Ab Initio Exciton and Phonon Dynamics in Transition Metal Dichalcogenides. ECS Meeting Abstracts, 2021, MA2021-01, 598-598.	0.0	0
12	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
13	Exploring the elastic and electronic properties of chromium molybdenum diboride alloys. Journal of Alloys and Compounds, 2021, 866, 158885.	5.5	8
14	Spontaneous interlayer compression in commensurately stacked van der Waals heterostructures. Physical Review B, 2021, 103, .	3.2	7
15	TB2J: A python package for computing magnetic interaction parameters. Computer Physics Communications, 2021, 264, 107938.	7.5	92
16	Gate Control of Spin-Layer-Locking FETs and Application to Monolayer LuIO. Nano Letters, 2021, 21, 7631-7636.	9.1	2
17	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
18	Electronic and Thermoelectric Properties of Transition-Metal Dichalcogenides. Journal of Physical Chemistry C, 2021, 125, 27084-27097.	3.1	21

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19	FrÃ¶hlich polaron effective mass and localization length in cubic materials: Degenerate and anisotropic electronic bands. Physical Review B, 2021, 104, .	3.2	8
20	The Abinitproject: Impact, environment and recent developments. Computer Physics Communications, 2020, 248, 107042.	7.5	369
21	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
22	Thermoelectric properties of elemental metals from first-principles electron-phonon coupling. Physical Review B, 2020, 102, .	3.2	13
23	Phonon-limited electron mobility in Si, GaAs, and GaP with exact treatment of dynamical quadrupoles. Physical Review B, 2020, 102, .	3.2	47
24	Electron-Phonon beyond FrÃ¶hlich: Dynamical Quadrupoles in Polar and Covalent Solids. Physical Review Letters, 2020, 125, 136601.	7.8	60
25	ABINIT: Overview and focus on selected capabilities. Journal of Chemical Physics, 2020, 152, 124102.	3.0	179
26	Direct time-domain determination of electron-phonon coupling strengths in chromium. Physical Review B, 2020, 102, .	3.2	4
27	(Invited) Ab Initio Exciton and Phonon Dynamics in Transition Metal Dichalcogenides. ECS Meeting Abstracts, 2020, MA2020-01, 749-749.	0.0	0
28	Surface Phonons: Theoretical Methods and Results. Springer Handbooks, 2020, , 737-782.	0.6	2
29	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
30	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
31	Spectroscopic properties of few-layer tin chalcogenides. JPhys Materials, 2019, 2, 044005.	4.2	12
32	Lattice dynamics and phase stability of rhombohedral antimony under high pressure. Physical Review B, 2019, 100, .	3.2	4
33	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
34	Density functional perturbation theory within noncollinear magnetism. Physical Review B, 2019, 99, .	3.2	8
35	The physics of single-side fluorination of graphene: DFT and DFTÂ+ U studies. Carbon, 2019, 144, 615-627.	10.3	30
36	Vibrational and dielectric properties of monolayer transition metal dichalcogenides. Physical Review Materials, 2019, 3, .	2.4	10

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37	The PseudoDojo: Training and grading a 85 element optimized norm-conserving pseudopotential table. Computer Physics Communications, 2018, 226, 39-54.	7.5	1,001
38	The psml format and library for norm-conserving pseudopotential data curation and interoperability. Computer Physics Communications, 2018, 227, 51-71.	7.5	38
39	Hybrid quantum anomalous Hall effect at graphene-oxide interfaces. Physical Review B, 2018, 98, .	3.2	10
40	From one to three, exploring the rungs of Jacobâ€™s ladder in magnetic alloys. European Physical Journal B, 2018, 91, 1.	1.5	15
41	BoltzTraP2, a program for interpolating band structures and calculating semi-classical transport coefficients. Computer Physics Communications, 2018, 231, 140-145.	7.5	730
42	Electron-Beam Manipulation of Silicon Dopants in Graphene. Nano Letters, 2018, 18, 5319-5323.	9.1	98
43	Competition of lattice and spin excitations in the temperature dependence of spin-wave properties. Physical Review B, 2018, 97, .	3.2	5
44	Vibrational and dielectric properties of the bulk transition metal dichalcogenides. Physical Review Materials, 2018, 2, .	2.4	25
45	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
46	Origin of the counterintuitive dynamic charge in the transition metal dichalcogenides. Physical Review B, 2017, 95, .	3.2	34
47	Zhao etÂal. Reply. Physical Review Letters, 2017, 118, 239602.	7.8	4
48	Conflicting evidence for ferroelectricity. Nature, 2017, 547, E9-E10.	27.8	10
49	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
50	First-Principles Study of the Thermoelectric Properties of SrRuO3. Journal of Physical Chemistry C, 2016, 120, 9112-9121.	3.1	27
51	Recent developments in the ABINIT software package. Computer Physics Communications, 2016, 205, 106-131.	7.5	662
52	Quasi-One-Dimensional Metal-Insulator Transitions in Compound Semiconductor Surfaces. Physical Review Letters, 2016, 117, 116101.	7.8	5
53	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></mml:math> Physical Review B, 2016, 94, .	3.2	23
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	High Temperature Ferromagnetism in a GdAg₂ Monolayer. Nano Letters, 2016, 16, 4230-4235.	9.1	40
56	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> from first principles and Seebeck local probes. Physical Review B, 2015, 92, .	3.2	9
57	Thermal conductivity in PbTe from first principles. Physical Review B, 2015, 91, .	3.2	98
58	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
59	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
60	Temperature dependence of the electronic structure of semiconductors and insulators. Journal of Chemical Physics, 2015, 143, 102813.	3.0	139
61	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
62	Ab initio calculation of the thermal conductivity of indium antimonide. Semiconductor Science and Technology, 2014, 29, 124002.	2.0	6
63	Cumulant expansion for phonon contributions to the electron spectral function. Physical Review B, 2014, 90, .	3.2	30
64	Are Hydrogen-Bonded Charge Transfer Crystals Room Temperature Ferroelectrics?. Physical Review Letters, 2014, 113, 237602.	7.8	35
65	First-principles study of the lattice dynamical properties of strontium ruthenate. Journal of Physics Condensed Matter, 2014, 26, 035401.	1.8	29
66	First Principles Explanation of the Positive Seebeck Coefficient of Lithium. Physical Review Letters, 2014, 112, 196603.	7.8	68
67	Role of Dynamical Instability in theAbÂInitioPhase Diagram of Calcium. Physical Review Letters, 2013, 111, 025503.	7.8	16
68	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
69	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
70	Ab initiocalculation of spin-dependent electronâ€“phonon coupling in iron and cobalt. Journal of Physics Condensed Matter, 2013, 25, 136001.	1.8	26
71	First-principles study of transport properties in Os and OsSi. Physical Review B, 2013, 87, .	3.2	12
72	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

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73	Implementation of density-functional perturbation theory within ABINIT: Projector augmented-waves and spin-orbit. AIP Conference Proceedings, 2012, , .	0.4	1
74	Thermopower in oxide heterostructures: The importance of being multiple-band conductors. Physical Review B, 2012, 86, .	3.2	48
75	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
76	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
77	Density functional theory beyond the linear regime: Validating an adiabatic local density approximation. Physical Review A, 2011, 83, .	2.5	61
78	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
79	Electronic properties of the Mg2Si thermoelectric material investigated by linear-response density-functional theory. Computational Materials Science, 2011, 50, 847-851.	3.0	46
80	A theoretical approach to ironâ€based superconductors. Annalen Der Physik, 2011, 523, 580-581.	2.4	0
81	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>. Physical Review Letters, 2010, 105, 016101.	7.8	22
82	Phases of Polonium via Density Functional Theory. Physical Review Letters, 2010, 104, 035501.	7.8	20
83	Demixing processes in AgPd superlattices. Journal of Physics Condensed Matter, 2009, 21, 315002.	1.8	5
84	ABINIT: First-principles approach to material and nanosystem properties. Computer Physics Communications, 2009, 180, 2582-2615.	7.5	2,297
85	First-principles conductance of nanoscale junctions from the polarizability of finite systems. Journal of Chemical Physics, 2009, 130, 124715.	3.0	7
86	Sharing electronic structure and crystallographic data with ETSF_IO. Computer Physics Communications, 2008, 179, 748-758.	7.5	9
87	Specification of an extensible and portable file format for electronic structure and crystallographic data. Computational Materials Science, 2008, 43, 1056-1065.	3.0	7
88	Density functional perturbation theory with spin-orbit coupling: Phonon band structure of lead. Physical Review B, 2008, 78, .	3.2	66
89	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
90	Phonon band structure and electron-phonon interactions in metallic nanowires. Physical Review B, 2006, 74, .	3.2	20

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91	Modeling the dissociation and ionization of a sputtered organic molecule. Applied Surface Science, 2006, 252, 6459-6462.	6.1	5
92	A brief introduction to the ABINIT software package. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.8	1,101
93	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
94	Why is iridium the best substrate for single crystal diamond growth?. Applied Physics Letters, 2005, 86, 191917.	3.3	26
95	Atomic structure of theTeâˆ•Si(100)â€(2Ã—1)surface. Physical Review B, 2005, 72, .	3.2	1
96	Structural and electronic properties ofAgâˆ’Pdsuperlattices. Physical Review B, 2004, 70, .	3.2	8
97	Anomalous ESR behavior of carbon nanofilaments grown from palladium seeds. Carbon, 2004, 42, 1049-1052.	10.3	17
98	Catalyst consumption during growth of carbon nanofilaments on Pd seeds. Applied Physics Letters, 2004, 85, 5376-5378.	3.3	2
99	Metals at finite temperature: a modified smearing scheme. Computational Materials Science, 2004, 30, 27-33.	3.0	3
100	Electronic structure of Agâ€“Pd heterostructures. Computational Materials Science, 2004, 30, 34-43.	3.0	3
101	First-principles calculation of the electronic, dielectric, and dynamical properties ofCaF2. Physical Review B, 2003, 68, .	3.2	62
102	Ab initiostudy ofMoS2nanotube bundles. Physical Review B, 2003, 68, .	3.2	27
103	First-principles computation of material properties: the ABINIT software project. Computational Materials Science, 2002, 25, 478-492.	3.0	2,789
104	Smearing scheme for finite-temperature electronic-structure calculations. Physical Review B, 2001, 65, .	3.2	32