Michel CÃ´tÃ©

List of Publications by Year
in descending order

85 papers	9,102 citations	117625 34 h-index	69250 77 g-index
88 all docs	88 docs citations	88 times ranked	9364 citing authors

#	Article	IF	Citations
1	Cubic spline solver for generalized density functional treatments of atoms and generation of atomic datasets for use with exchange-correlation functionals including meta-GGA. Physical Review B, 2022, 105, .	3.2	9
2	Visible Out-of-plane Polarized Luminescence and Electronic Resonance in Black Phosphorus. Nano Letters, 2022, , .	9.1	5
3	Longitudinal piezoelectric, elastic, and dielectric properties of rare-earth aluminum nitride alloys determined by density-functional perturbation theory. Physical Review Materials, 2022, 6, .	2.4	2
4	Impact of applied biaxial stress on the piezoelectric, elastic, and dielectric properties of scandium aluminum nitride alloys determined by density functional perturbation theory. AIP Advances, 2021, 11, .	1.3	3
5	Influence of the Electronâ€“Phonon Interaction on the Topological Phase Transition in BiTeI. , 2021, , 305-313.		0
6	FrÃ¶hlich polaron effective mass and localization length in cubic materials: Degenerate and anisotropic electronic bands. Physical Review B, 2021, 104, .	3.2	8
7	The Abinitproject: Impact, environment and recent developments. Computer Physics Communications, 2020, 248, 107042.	7.5	369
8	Predominance of non-adiabatic effects in zero-point renormalization of the electronic band gap. Npj Computational Materials, 2020, 6, .	8.7	65
9	ABINIT: Overview and focus on selected capabilities. Journal of Chemical Physics, 2020, 152, 124102.	3.0	179
10	Ab initio piezoelectric properties of wurtzite ZnO-based alloys: Impact of the c/a cell ratio. Physical Review Materials, 2020, 4, .	2.4	4
11	Temperature dependence of the topological phase transition of BiTeI from first principles. Physical Review Research, 2020, 2, .	3.6	11
12	(Invited) Momentum-Resolved Dielectric Response of Free Standing Black Phosphorus Down to the Monolayer. ECS Meeting Abstracts, 2020, MA2020-01, 840-840.	0.0	0
13	(Invited) Dynamics of Nitrogen Functionalization of Graphene. ECS Meeting Abstracts, 2020, MA2020-01, 735-735.	0.0	0
14	Momentum-Resolved Dielectric Response of Free-Standing Mono-, Bi-, and Trilayer Black Phosphorus. Nano Letters, 2019, 19, 8303-8310.	9.1	27
15	Charge fluctuations in lightly hole-doped cuprates: Effect of vertex corrections. Physical Review B, 2019, 99, .	3.2	16
16	Superconducting Symmetries of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Sr</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow><mml:mn></mml:mn></mml:msub></mml:mrow></mml:math> from First-Principles Electronic Structure. Physical Review Letters, 2019, 123, 217005.	7.8	47
17	Unconventional field induced phases in a quantum magnet formed by free radical tetramers. Physical Review B, 2018, 97, .	3.2	5
18	Second-Order Raman Scattering in Exfoliated Black Phosphorus. Nano Letters, 2018, 18, 1018-1027.	9.1	32

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19	Antiresonances in the Mid-Infrared Vibrational Spectrum of Functionalized Graphene. Journal of Physical Chemistry C, 2017, 121, 9053-9062.	3.1	7
20	Ab initio piezoelectric properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Al</mml:mi><mml:mrow><mml:mn>0.5</mml:mn></mml:mrow></mml:msub><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math> : Impact of alloy configuration on the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>d</mml:mi><mml:mrow><mml:mn>33</mml:mn></mml:mrow></mml:msub></mml:math> Physical Review Materials, 2017, 1, .	2.4	18
21	(Invited) Probing the Dielectric Response of Exfoliated Black Phosphorous in Free Standing Conditions. ECS Meeting Abstracts, 2017, , .	0.0	0
22	Phonon and Defect Induced Transparencies in the Mid-Infrared Spectrum of Grafted Single Layer Graphene. ECS Meeting Abstracts, 2017, , .	0.0	0
23	Recent developments in the ABINIT software package. Computer Physics Communications, 2016, 205, 106-131.	7.5	662
24	Na 3 Fe 2 (SO 4) 2 (SO 3 N) as a potential high capacity cathode material. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2016, 211, 185-190.	3.5	1
25	Dynamical and anharmonic effects on the electron-phonon coupling and the zero-point renormalization of the electronic structure. Physical Review B, 2015, 92, .	3.2	104
26	Fermi surface of the superconductorBaIr2P2. Physical Review B, 2015, 92, .	3.2	5
27	Resonance Raman spectroscopy and imaging of pushâ€“pull conjugated polymerâ€“fullerene blends. Journal of Materials Chemistry C, 2015, 3, 6058-6066.	5.5	24
28	A novel intercalation cathode material for sodium-based batteries. Electrochemistry Communications, 2015, 52, 9-12.	4.7	1
29	Graft-Induced Midgap States in Functionalized Carbon Nanotubes. ACS Nano, 2015, 9, 2626-2634.	14.6	13
30	Efficient dielectric matrix calculations using the Lanczos algorithm for fast many-body<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2015, 91, .	3.2	18
31	Temperature dependence of electronic eigenenergies in the adiabatic harmonic approximation. Physical Review B, 2014, 90, .	3.2	91
32	GaAs-δ layered within nitrogen for high efficiency photovoltaic devices: First principle prediction. , 2014, , .		0
33	Many-Body Effects on the Zero-Point Renormalization of the Band Structure. Physical Review Letters, 2014, 112, .	7.8	141
34	Verification of first-principles codes: Comparison of total energies, phonon frequencies, electronâ€“phonon coupling and zero-point motion correction to the gap between ABINIT and QE/Yambo. Computational Materials Science, 2014, 83, 341-348.	3.0	88
35	Thiocarbonyl Substitution in 1,4-Dithioketopyrrolopyrrole and Thienopyrroledithione Derivatives: An Experimental and Theoretical Study. Journal of Physical Chemistry C, 2014, 118, 3953-3959.	3.1	19
36	Fermi-surface topology of the iron pnictide<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>LaFe</mml:mtext><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mtext>P</mml:mtext><mml:mn>2</mml:mn></mml:msub></mml:math> Physical Review B, 2014, 89, .	3.2	8

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37	Direct observation of ultrafast long-range charge separation at polymerâ€“fullerene heterojunctions. Nature Communications, 2014, 5, 4288.	12.8	140
38	Low Band Gap Polymers Design Approach Based on a Mix of Aromatic and Quinoid Structures. Macromolecules, 2013, 46, 6873-6880.	4.8	36
39	Bromophenyl functionalization of carbon nanotubes: an ab initio study. Nanotechnology, 2013, 24, 375702.	2.6	5
40	Two-dimensional spatial coherence of excitons in semicrystalline polymeric semiconductors: Effect of molecular weight. Physical Review B, 2013, 88, .	3.2	96
41	Designing Polymers for Photovoltaic Applications Using ab Initio Calculations. Journal of Physical Chemistry C, 2013, 117, 7964-7972.	3.1	62
42	Fermi-surface evolution in Yb-substituted CeCoIn5. Physical Review B, 2012, 85, .	3.2	26
43	Large electronic bandwidth in solution-processable pyrene crystals: The role of close-packed crystal structure. Journal of Chemical Physics, 2012, 137, 034706.	3.0	10
44	Effects of plasmon pole models on the G0W0 electronic structure of various oxides. European Physical Journal B, 2012, 85, 1.	1.5	24
45	Enhanced electron-phonon coupling near the lattice instability of superconducting NbC<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<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>from density-functional calculations. Physical Review B, 2011, 84, .	3.2	23
46	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mml:msup><mml:msup><mml:mi>W</mml:mi><mml:mn>0</mml:mn></mml:msup></mml:mrow></mml:math> gap of ZnO: Effects of plasmon-pole models. Physical Review B, 2011, 84, .	3.2	102
47	Electron-phonon coupling in the C60fullerene within the many-bodyGWapproach. Physical Review B, 2011, 84, .	3.2	82
48	Theoretical approaches to the temperature and zeroâ€point motion effects on the electronic band structure. Annalen Der Physik, 2011, 523, 168-178.	2.4	81
49	DFT‐GGA+<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>U</mml:mi></mml:math>study of magnetic order in doped La<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>CuO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>crystals. Physical Review B, 2011, 84, .	3.2	22
50	Peierls instability in carbon nanotubes: A first-principles study. Physical Review B, 2010, 82, .	3.2	25
51	Electron-phonon coupling in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>C</mml:mtext><mml:mrow><mml:mn>60</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>: hybrid functionals. Physical Review B, 2010, 81, .	3.2	43
52	Ab initiohigh-energy excitonic effects in graphite and graphene. Physical Review B, 2010, 81, .	3.2	77
53	Doping ofC60-induced electronic states in BN nanopeapods:Ab initiosimulations. Physical Review B, 2009, 80, .	3.2	6
54	First principles elaboration of low band gap ladder-type polymers. Journal of Chemical Physics, 2009, 130, 114906.	3.0	6

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55	ABINIT: First-principles approach to material and nanosystem properties. Computer Physics Communications, 2009, 180, 2582-2615.	7.5	2,297
56	Excitons in perylene tetracarboxdiimide crystals for optoelectronics. Physica Status Solidi C: Current Topics in Solid State Physics, 2009, 6, 93-96.	0.8	3
57	Ab initio study of ladder-type polymers: Polythiophene and polypyrrole. Chemical Physics Letters, 2008, 450, 329-334.	2.6	25
58	Nitrogen incorporation and lattice constant of strained diluteGaAs1âˆ'xNxlayers on GaAs (001): Anab initiostudy. Physical Review B, 2006, 74, .	3.2	11
59	Experimental and theoretical studies of theE+optical transition inGaAsNalloys. Physical Review B, 2006, 74, .	3.2	13
60	Fullerene in a Metal-Organic Matrix: Design of the Electronic Structure. Physical Review Letters, 2005, 95, 146403.	7.8	15
61	Raman study of optical phonons in ultrathinInAsâ•InPsingle strained quantum wells. Physical Review B, 2005, 72, .	3.2	3
62	Theory of Tunnel Ionization in Complex Systems. Physical Review Letters, 2005, 95, 073001.	7.8	84
63	A first principles calculations and experimental study of the ground- and excited-state properties of ladder oligo(p-aniline)s. Journal of Chemical Physics, 2005, 122, 104303.	3.0	29
64	Evidence for large configuration-induced band-gap fluctuations inGaAs1âˆ'xNxalloys. Physical Review B, 2004, 70, .	3.2	21
65	Structural Relaxations in Electronically Excited Poly(para-phenylene). Physical Review Letters, 2004, 93, 116401.	7.8	49
66	First-principles study of the rotational transitions of H[sub 2] physisorbed over benzene. Journal of Chemical Physics, 2004, 121, 12618.	3.0	40
67	Electronic, Structural, and Optical Properties of Conjugated Polymers Based on Carbazole, Fluorene, and Borafluorene. Journal of Physical Chemistry B, 2004, 108, 3123-3129.	2.6	71
68	Ab initio study of the hindered rotation of H2 over benzene. Materials Research Society Symposia Proceedings, 2003, 801, 7.	0.1	0
69	Material design from first principles: the case of boron nitride polymers. Journal of Physics Condensed Matter, 2002, 14, 9997-10009.	1.8	6
70	Boron nitride polymers: Building blocks for organic electronic devices. Physical Review B, 2001, 63, .	3.2	43
71	Parallel fast Fourier transforms for electronic structure calculations. Computer Physics Communications, 2000, 130, 130-136.	7.5	21
72	Scanning Tunneling Spectroscopy ofC36. Physical Review Letters, 1999, 82, 165-168.	7.8	77

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73	Transition metals and their carbides and nitrides: â€ƒTrends in electronic and structural properties. Physical Review B, 1999, 60, 6343-6347.	3.2	236
74	Electronic and structural properties of molecular C36. Chemical Physics Letters, 1998, 284, 344-349.	2.6	106
75	Theoretical study of a three-dimensional all-sp2structure. Physical Review B, 1998, 58, 664-668.	3.2	47
76	Theoretical study of the structural and electronic properties of GaSe nanotubes. Physical Review B, 1998, 58, R4277-R4280.	3.2	129
77	Band structures of CsCl-structured BaS and CaSe at high pressure: Implications for metallization pressures of the alkaline earth chalcogenides. Physical Review B, 1998, 58, 9793-9800.	3.2	37
78	Electron-Phonon Interactions in SolidC36. Physical Review Letters, 1998, 81, 697-700.	7.8	136
79	Carbon nitride compounds with 1:1 stoichiometry. Physical Review B, 1997, 55, 5684-5688.	3.2	32
80	Ab initio calculations of the pressure-induced structural phase transitionsfor four II-VI compounds. Physical Review B, 1997, 55, 13025-13031.	3.2	191
81	Ab initiostudy of silicon in theR8phase. Physical Review B, 1997, 56, 6662-6668.	3.2	103
82	Relaxation of Crystals with the Quasi-Newton Method. Journal of Computational Physics, 1997, 131, 233-240.	3.8	2,389
83	Band structure of CdS and CdSe at high pressure. Physical Review B, 1996, 54, 17585-17590.	3.2	35
84	Balanced 6 Ã— 6 designs for 4 equally replicated treatments. Discrete Mathematics, 1994, 125, 319-327.	0.7	1
85	Energy bounds for the generalized exponentialâ€“cosine screened Coulomb potential. Canadian Journal of Physics, 1994, 72, 233-237.	1.1	0