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	Relaxation of Crystals with the Quasi-Newton Method. Journal of Computational Physics, 1997, 131, 233-240.	3.8	2,389
2	ABINIT: First-principles approach to material and nanosystem properties. Computer Physics Communications, 2009, 180, 2582-2615.	7.5	2,297
3	Recent developments in the ABINIT software package. Computer Physics Communications, 2016, 205, 106-131.	7.5	662
4	The Abinitproject: Impact, environment and recent developments. Computer Physics Communications, 2020, 248, 107042.	7.5	369
5	Transition metals and their carbides and nitrides: â€ƒTrends in electronic and structural properties. Physical Review B, 1999, 60, 6343-6347.	3.2	236
6	Ab initio calculations of the pressure-induced structural phase transitionsfor four II-VI compounds. Physical Review B, 1997, 55, 13025-13031.	3.2	191
7	ABINIT: Overview and focus on selected capabilities. Journal of Chemical Physics, 2020, 152, 124102.	3.0	179
8	Many-Body Effects on the Zero-Point Renormalization of the Band Structure. Physical Review Letters, 2014, 112, .	7.8	141
9	Direct observation of ultrafast long-range charge separation at polymerâ€“fullerene heterojunctions. Nature Communications, 2014, 5, 4288.	12.8	140
10	Electron-Phonon Interactions in SolidC36. Physical Review Letters, 1998, 81, 697-700.	7.8	136
11	Theoretical study of the structural and electronic properties of GaSe nanotubes. Physical Review B, 1998, 58, R4277-R4280.	3.2	129
12	Electronic and structural properties of molecular C36. Chemical Physics Letters, 1998, 284, 344-349.	2.6	106
13	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
14	Ab initiostudy of silicon in theR8phase. Physical Review B, 1997, 56, 6662-6668.	3.2	103
15	<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> gap of ZnO: Effects of plasmon-pole models. Physical Review B, 2011, 84, .	3.2	101
16	Two-dimensional spatial coherence of excitons in semicrystalline polymeric semiconductors: Effect of molecular weight. Physical Review B, 2013, 88, .	3.2	96
17	Temperature dependence of electronic eigenenergies in the adiabatic harmonic approximation. Physical Review B, 2014, 90, .	3.2	91
18	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

#	ARTICLE	IF	CITATIONS
19	Theory of Tunnel Ionization in Complex Systems. Physical Review Letters, 2005, 95, 073001.	7.8	84
20	Electron-phonon coupling in the C60fullerene within the many-bodyGWapproach. Physical Review B, 2011, 84, .	3.2	82
21	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
22	Scanning Tunneling Spectroscopy ofC36. Physical Review Letters, 1999, 82, 165-168.	7.8	77
23	Ab initiohigh-energy excitonic effects in graphite and graphene. Physical Review B, 2010, 81, .	3.2	77
24	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
25	Predominance of non-adiabatic effects in zero-point renormalization of the electronic band gap. Npj Computational Materials, 2020, 6, .	8.7	65
26	Designing Polymers for Photovoltaic Applications Using ab Initio Calculations. Journal of Physical Chemistry C, 2013, 117, 7964-7972.	3.1	62
27	Structural Relaxations in Electronically Excited Poly(para-phenylene). Physical Review Letters, 2004, 93, 116401.	7.8	49
28	Theoretical study of a three-dimensional all-sp2structure. Physical Review B, 1998, 58, 664-668.	3.2	47
29	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> from First-Principles Electronic Structure. Physical Review Letters, 2019, 123, 217005.	7.8	47
30	Boron nitride polymers: Building blocks for organic electronic devices. Physical Review B, 2001, 63, .	3.2	43
31	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> hybrid functionals. Physical Review B, 2010, 81, .	3.2	43
32	First-principles study of the rotational transitions of H[sub 2] physisorbed over benzene. Journal of Chemical Physics, 2004, 121, 12618.	3.0	40
33	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
34	Low Band Gap Polymers Design Approach Based on a Mix of Aromatic and Quinoid Structures. Macromolecules, 2013, 46, 6873-6880.	4.8	36
35	Band structure of CdS and CdSe at high pressure. Physical Review B, 1996, 54, 17585-17590.	3.2	35
36	Carbon nitride compounds with 1:1 stoichiometry. Physical Review B, 1997, 55, 5684-5688.	3.2	32

#	Article	IF	Citations
37	Second-Order Raman Scattering in Exfoliated Black Phosphorus. Nano Letters, 2018, 18, 1018-1027.	9.1	32
38	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
39	Momentum-Resolved Dielectric Response of Free-Standing Mono-, Bi-, and Trilayer Black Phosphorus. Nano Letters, 2019, 19, 8303-8310.	9.1	27
40	Fermi-surface evolution in Yb-substituted CeCoIn5. Physical Review B, 2012, 85, .	3.2	26
41	Ab initio study of ladder-type polymers: Polythiophene and polypyrrole. Chemical Physics Letters, 2008, 450, 329-334.	2.6	25
42	Peierls instability in carbon nanotubes: A first-principles study. Physical Review B, 2010, 82, .	3.2	25
43	Effects of plasmon pole models on the G0W0 electronic structure of various oxides. European Physical Journal B, 2012, 85, 1.	1.5	24
44	Resonance Raman spectroscopy and imaging of pushâ€“pull conjugated polymerâ€“fullerene blends. Journal of Materials Chemistry C, 2015, 3, 6058-6066.	5.5	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:mrow><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math> from DFTâ€“â€“LDA calculations. Physical Review B, 2011, 84, .	3.2	23
46	<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
47	Parallel fast Fourier transforms for electronic structure calculations. Computer Physics Communications, 2000, 130, 130-136.	7.5	21
48	Evidence for large configuration-induced band-gap fluctuations inGaAs1âˆ’xNxalloys. Physical Review B, 2004, 70, .	3.2	21
49	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
50	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
51	First-principles prediction of 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: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:math> Physical Review Materials, 2017, 1, .	2.4	18
52	Charge fluctuations in lightly hole-doped cuprates: Effect of vertex corrections. Physical Review B, 2019, 99, .	3.2	16
53	Fullerene in a Metal-Organic Matrix: Design of the Electronic Structure. Physical Review Letters, 2005, 95, 146403.	7.8	15
54	Experimental and theoretical studies of theE+optical transition inGaAsNalloys. Physical Review B, 2006, 74, .	3.2	13

#	ARTICLE	IF	CITATIONS
55	Graft-Induced Midgap States in Functionalized Carbon Nanotubes. ACS Nano, 2015, 9, 2626-2634.	14.6	13
56	Nitrogen incorporation and lattice constant of strained diluteGaAs1âˆ’xNxlayers on GaAs (001): Anab initiostudy. Physical Review B, 2006, 74, .	3.2	11
57	Temperature dependence of the topological phase transition of BiTeI from first principles. Physical Review Research, 2020, 2, .	3.6	11
58	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
59	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
60	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
61	FrÃ¶hlich polaron effective mass and localization length in cubic materials: Degenerate and anisotropic electronic bands. Physical Review B, 2021, 104, .	3.2	8
62	Antiresonances in the Mid-Infrared Vibrational Spectrum of Functionalized Graphene. Journal of Physical Chemistry C, 2017, 121, 9053-9062.	3.1	7
63	Material design from first principles: the case of boron nitride polymers. Journal of Physics Condensed Matter, 2002, 14, 9997-10009.	1.8	6
64	Doping ofC60-induced electronic states in BN nanopeapods:Ab initiosimulations. Physical Review B, 2009, 80, .	3.2	6
65	First principles elaboration of low band gap ladder-type polymers. Journal of Chemical Physics, 2009, 130, 114906.	3.0	6
66	Bromophenyl functionalization of carbon nanotubes: an ab initio study. Nanotechnology, 2013, 24, 375702.	2.6	5
67	Fermi surface of the superconductorBaIr2P2. Physical Review B, 2015, 92, .	3.2	5
68	Unconventional field induced phases in a quantum magnet formed by free radical tetramers. Physical Review B, 2018, 97, .	3.2	5
69	Visible Out-of-plane Polarized Luminescence and Electronic Resonance in Black Phosphorus. Nano Letters, 2022, , .	9.1	5
70	Ab initio piezoelectric properties of wurtzite ZnO-based alloys: Impact of the c/a cell ratio. Physical Review Materials, 2020, 4, .	2.4	4
71	Raman study of optical phonons in ultrathinInAsâ•InPsingle strained quantum wells. Physical Review B, 2005, 72, .	3.2	3
72	Excitons in perylene tetracarboxdiimide crystals for optoelectronics. Physica Status Solidi C: Current Topics in Solid State Physics, 2009, 6, 93-96.	0.8	3

#	Article	IF	Citations
73	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
74	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
75	Balanced 6 Ã— 6 designs for 4 equally replicated treatments. Discrete Mathematics, 1994, 125, 319-327.	0.7	1
76	A novel intercalation cathode material for sodium-based batteries. Electrochemistry Communications, 2015, 52, 9-12.	4.7	1
77	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
78	Energy bounds for the generalized exponentialâ€“cosine screened Coulomb potential. Canadian Journal of Physics, 1994, 72, 233-237.	1.1	0
79	Ab initio study of the hindered rotation of H2 over benzene. Materials Research Society Symposia Proceedings, 2003, 801, 7.	0.1	0
80	GaAs-δ layered within nitrogen for high efficiency photovoltaic devices: First principle prediction. , 2014, , .		0
81	(Invited) Probing the Dielectric Response of Exfoliated Black Phosphorous in Free Standing Conditions. ECS Meeting Abstracts, 2017, , .	0.0	0
82	Phonon and Defect Induced Transparencies in the Mid-Infrared Spectrum of Grafted Single Layer Graphene. ECS Meeting Abstracts, 2017, , .	0.0	0
83	(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
84	(Invited) Dynamics of Nitrogen Functionalization of Graphene. ECS Meeting Abstracts, 2020, MA2020-01, 735-735.	0.0	0
85	Influence of the Electronâ€“Phonon Interaction on the Topological Phase Transition in BiTeI. , 2021, , 305-313.		0