Damien Caliste

List of Publications by Year
in descending order

45	5,994	304743	243625
papers	citations	22 h-index	44 g-index

49	49	49	7609
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	ABINIT: First-principles approach to material and nanosystem properties. Computer Physics Communications, 2009, 180, 2582-2615.	7.5	2,297
2	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
3	Recent developments in the ABINIT software package. Computer Physics Communications, 2016, 205, 106-131.	7.5	662
4	Crystal Structure of Cold Compressed Graphite. Physical Review Letters, 2012, 108, 065501.	7.8	292
5	Daubechies wavelets as a basis set for density functional pseudopotential calculations. Journal of Chemical Physics, 2008, 129, 014109.	3.0	289
6	ABINIT: Overview and focus on selected capabilities. Journal of Chemical Physics, 2020, 152, 124102.	3.0	179
7	Accurate and efficient linear scaling DFT calculations with universal applicability. Physical Chemistry Chemical Physics, 2015, 17, 31360-31370.	2.8	158
8	Daubechies wavelets for linear scaling density functional theory. Journal of Chemical Physics, 2014, 140, 204110.	3.0	140
9	Optimized energy landscape exploration using the ab initio based activation-relaxation technique. Journal of Chemical Physics, 2011, 135, 034102.	3.0	81
10	Single artificial atoms in silicon emitting at telecom wavelengths. Nature Electronics, 2020, 3, 738-743.	26.0	72
11	Impact of isovalent doping on the trapping of vacancy and interstitial related defects in Si. Journal of Applied Physics, 2013, 113, 113506.	2.5	61
12	Flexibilities of wavelets as a computational basis set for large-scale electronic structure calculations. Journal of Chemical Physics, 2020, 152, 194110.	3.0	60
13	Phase diagram, structure, and magnetic properties of the Ge-Mn system: A first-principles study. Physical Review B, 2011, 83, .	3.2	47
14	Toward the IIIâ€“V/Si co-integration by controlling the biatomic steps on hydrogenated Si(001). Applied Physics Letters, 2016, 109, .	3.3	46
15	Vacancy-Assisted Diffusion in Silicon: A Three-Temperature-Regime Model. Physical Review Letters, 2006, 97, 135901.	7.8	44
16	Synchrotron Bragg diffraction imaging characterization of synthetic diamond crystals for optical and electronic power device applications. Journal of Applied Crystallography, 2017, 50, 561-569.	4.5	39
17	First-principles prediction of stable SiC cage structures and their synthesis pathways. Physical Review B, 2010, 82, .	3.2	37
18	Low-energy boron fullerenes: Role of disorder and potential synthesis pathways. Physical Review B, 2011, 83, .	3.2	37

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19	Germanium diffusion mechanisms in silicon from first principles. Physical Review B, 2007, 75, .	3.2	33
20	Revisiting the domain model for lithium intercalated graphite. Applied Physics Letters, 2013, 103, .	3.3	33
21	Mg and In Codoped p-type AlN Nanowires for pn Junction Realization. Nano Letters, 2019, 19, 8357-8364.	9.1	25
22	Superglide at an Internal Incommensurate Boundary. Nano Letters, 2010, 10, 695-700.	9.1	23
23	Efficient Computation of Sparse Matrix Functions for Large-Scale Electronic Structure Calculations: The <scp>CheSS</scp> Library. Journal of Chemical Theory and Computation, 2017, 13, 4684-4698.	5.3	23
24	Thermodynamics and Related Kinetics of Staging in Intercalation Compounds. Journal of Physical Chemistry C, 2019, 123, 23711-23720.	3.1	22
25	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	3.0	19
26	Point defect diffusion in Si and SiGe revisited through atomistic simulations. Materials Science in Semiconductor Processing, 2012, 15, 675-690.	4.0	18
27	A wavelet-based Projector Augmented-WaveÂ(PAW) method: Reaching frozen-core all-electron precision with a systematic, adaptive and localized wavelet basis set. Computer Physics Communications, 2016, 208, 1-8.	7.5	18
28	Structural, electronic, and optical properties of the C-C complex in bulk silicon from first principles. Journal of Applied Physics, 2018, 123, .	2.5	16
29	Interface identification of the solid electrolyte interphase on graphite. Carbon, 2017, 111, 789-795.	10.3	15
30	Passivation mechanism in CdTe solar cells: The hybrid role of Se. Applied Physics Letters, 2021, 119, .	3.3	12
31	First principles prediction of the metastability of the Ge2Mn phase and its synthesis pathways. Applied Physics Letters, 2010, 96, 231904.	3.3	11
32	Vacancy-mediated diffusion in biaxially strained Si. Applied Physics Letters, 2011, 98, 031908.	3.3	11
33	Sharing electronic structure and crystallographic data with ETSF_IO. Computer Physics Communications, 2008, 179, 748-758.	7.5	9
34	Deciphering mechanisms of enhanced-retarded oxygen diffusion in doped Si. Applied Physics Letters, 2013, 103, .	3.3	9
35	Specification of an extensible and portable file format for electronic structure and crystallographic data. Computational Materials Science, 2008, 43, 1056-1065.	3.0	7
36	Rocking Curve Imaging Investigation of the Long-Range Distortion Field between Parallel Dislocations with Opposite Burgers Vectors. Applied Sciences (Switzerland), 2021, 11, 9054.	2.5	6

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37	Hole- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mi mathvariant="normal">Cr</mml:mi><mml:mo>+</mml:mo></mml:msup></mml:math> nanomagnet in a semiconductor quantum dot. Physical Review B, 2021, 104, .	3.2	5
38	An atomistic vision of the Mass Action Law: Prediction of carbon/oxygen defects in silicon. Journal of Applied Physics, 2015, 118, .	2.5	4
39	Structure of an incommensurate 90Â° Si grain boundary resolved with the help of a Cs-corrector for illumination. Journal of Physics: Conference Series, 2010, 209, 012041.	0.4	3
40	Lattice vacancies in silicon film exposed to external electric field. Journal of Applied Physics, 2013, 114, 043713.	2.5	3
41	Charge distribution and chemical bonding in B-O complexes in Cz-Si solar cells. Journal of Applied Physics, 2013, 114, 153708.	2.5	2
42	Oxygen in silicon: Switch in the diffusion-mediated mechanism. Physical Review B, 2017, 96, .	3.2	2
43	Correlation between Atomic Structure and Superglide of an Incommensurate Grain Boundary in Au. Microscopy and Microanalysis, 2010, 16, 1442-1443.	0.4	0
44	Response to â€œComment on â€˜Structural, electronic, and optical properties of the C-C complex in bulk silicon from first principlesâ€™â€•[J. Appl. Phys. 124, 086101 (2018)]. Journal of Applied Physics, 2018, 124, 086102.	2.5	0
45	Incommensurate grain boundary in silicon and the silver-ratio sequence. Physical Review B, 2019, 100, .	3.2	0