Damien Caliste

List of Publications by Year
in descending order

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45 papers	5,994 citations	304602 22 h-index	243529 44 g-index
49 all docs	49 docs citations	49 times ranked	7609 citing authors

#	Article	IF	Citations
1	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, .	1.1	5
2	Passivation mechanism in CdTe solar cells: The hybrid role of Se. Applied Physics Letters, 2021, 119, .	1.5	12
3	Rocking Curve Imaging Investigation of the Long-Range Distortion Field between Parallel Dislocations with Opposite Burgers Vectors. Applied Sciences (Switzerland), 2021, 11, 9054.	1.3	6
4	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	1.2	19
5	Single artificial atoms in silicon emitting at telecom wavelengths. Nature Electronics, 2020, 3, 738-743.	13.1	72
6	Flexibilities of wavelets as a computational basis set for large-scale electronic structure calculations. Journal of Chemical Physics, 2020, 152, 194110.	1.2	60
7	ABINIT: Overview and focus on selected capabilities. Journal of Chemical Physics, 2020, 152, 124102.	1.2	179
8	Mg and In Codoped p-type AlN Nanowires for pn Junction Realization. Nano Letters, 2019, 19, 8357-8364.	4.5	25
9	Thermodynamics and Related Kinetics of Staging in Intercalation Compounds. Journal of Physical Chemistry C, 2019, 123, 23711-23720.	1.5	22
10	Incommensurate grain boundary in silicon and the silver-ratio sequence. Physical Review B, 2019, 100, .	1.1	0
11	Structural, electronic, and optical properties of the C-C complex in bulk silicon from first principles. Journal of Applied Physics, 2018, 123, .	1.1	16
12	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.	1.1	0
13	Synchrotron Bragg diffraction imaging characterization of synthetic diamond crystals for optical and electronic power device applications. Journal of Applied Crystallography, 2017, 50, 561-569.	1.9	39
14	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.	2.3	23
15	Oxygen in silicon: Switch in the diffusion-mediated mechanism. Physical Review B, 2017, 96, .	1.1	2
16	Interface identification of the solid electrolyte interphase on graphite. Carbon, 2017, 111, 789-795.	5.4	15
17	Toward the IIIâ€“V/Si co-integration by controlling the biatomic steps on hydrogenated Si(001). Applied Physics Letters, 2016, 109, .	1.5	46
18	Recent developments in the ABINIT software package. Computer Physics Communications, 2016, 205, 106-131.	3.0	662

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19	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.	3.0	18
20	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
21	An atomistic vision of the Mass Action Law: Prediction of carbon/oxygen defects in silicon. Journal of Applied Physics, 2015, 118, .	1.1	4
22	Accurate and efficient linear scaling DFT calculations with universal applicability. Physical Chemistry Chemical Physics, 2015, 17, 31360-31370.	1.3	158
23	Daubechies wavelets for linear scaling density functional theory. Journal of Chemical Physics, 2014, 140, 204110.	1.2	140
24	Lattice vacancies in silicon film exposed to external electric field. Journal of Applied Physics, 2013, 114, 043713.	1.1	3
25	Charge distribution and chemical bonding in B-O complexes in Cz-Si solar cells. Journal of Applied Physics, 2013, 114, 153708.	1.1	2
26	Impact of isovalent doping on the trapping of vacancy and interstitial related defects in Si. Journal of Applied Physics, 2013, 113, 113506.	1.1	61
27	Deciphering mechanisms of enhanced-retarded oxygen diffusion in doped Si. Applied Physics Letters, 2013, 103, .	1.5	9
28	Revisiting the domain model for lithium intercalated graphite. Applied Physics Letters, 2013, 103, .	1.5	33
29	Point defect diffusion in Si and SiGe revisited through atomistic simulations. Materials Science in Semiconductor Processing, 2012, 15, 675-690.	1.9	18
30	Crystal Structure of Cold Compressed Graphite. Physical Review Letters, 2012, 108, 065501.	2.9	292
31	Low-energy boron fullerenes: Role of disorder and potential synthesis pathways. Physical Review B, 2011, 83, .	1.1	37
32	Phase diagram, structure, and magnetic properties of the Ge-Mn system: A first-principles study. Physical Review B, 2011, 83, .	1.1	47
33	Vacancy-mediated diffusion in biaxially strained Si. Applied Physics Letters, 2011, 98, 031908.	1.5	11
34	Optimized energy landscape exploration using the ab initio based activation-relaxation technique. Journal of Chemical Physics, 2011, 135, 034102.	1.2	81
35	Correlation between Atomic Structure and Superglide of an Incommensurate Grain Boundary in Au. Microscopy and Microanalysis, 2010, 16, 1442-1443.	0.2	0
36	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.	0.3	3

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37	First principles prediction of the metastability of the Ge2Mn phase and its synthesis pathways. Applied Physics Letters, 2010, 96, 231904.	1.5	11
38	First-principles prediction of stable SiC cage structures and their synthesis pathways. Physical Review B, 2010, 82, .	1.1	37
39	Superglide at an Internal Incommensurate Boundary. Nano Letters, 2010, 10, 695-700.	4.5	23
40	ABINIT: First-principles approach to material and nanosystem properties. Computer Physics Communications, 2009, 180, 2582-2615.	3.0	2,297
41	Sharing electronic structure and crystallographic data with ETSF_IO. Computer Physics Communications, 2008, 179, 748-758.	3.0	9
42	Specification of an extensible and portable file format for electronic structure and crystallographic data. Computational Materials Science, 2008, 43, 1056-1065.	1.4	7
43	Daubechies wavelets as a basis set for density functional pseudopotential calculations. Journal of Chemical Physics, 2008, 129, 014109.	1.2	289
44	Germanium diffusion mechanisms in silicon from first principles. Physical Review B, 2007, 75, .	1.1	33
45	Vacancy-Assisted Diffusion in Silicon: A Three-Temperature-Regime Model. Physical Review Letters, 2006, 97, 135901.	2.9	44