

Damien Caliste

List of Publications by Year in descending order

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papers

5,994
citations

304743

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243625

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49
all docs

49
docs citations

49
times ranked

7609
citing authors

#	ARTICLE	IF	CITATIONS
1	Hole- Cr^+ nanomagnet in a semiconductor quantum dot. Physical Review B, 2021, 104, .	3.2	5
2	Passivation mechanism in CdTe solar cells: The hybrid role of Se. Applied Physics Letters, 2021, 119, .	3.3	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.	2.5	6
4	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	3.0	19
5	Single artificial atoms in silicon emitting at telecom wavelengths. Nature Electronics, 2020, 3, 738-743.	26.0	72
6	Flexibilities of wavelets as a computational basis set for large-scale electronic structure calculations. Journal of Chemical Physics, 2020, 152, 194110.	3.0	60
7	ABINIT: Overview and focus on selected capabilities. Journal of Chemical Physics, 2020, 152, 124102.	3.0	179
8	Mg and In Codoped p-type AlN Nanowires for pn Junction Realization. Nano Letters, 2019, 19, 8357-8364.	9.1	25
9	Thermodynamics and Related Kinetics of Staging in Intercalation Compounds. Journal of Physical Chemistry C, 2019, 123, 23711-23720.	3.1	22
10	Incommensurate grain boundary in silicon and the silver-ratio sequence. Physical Review B, 2019, 100, .	3.2	0
11	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
12	Response to "Comment on "Structural, electronic, and optical properties of the C-C complex in bulk silicon from first principles" [J. Appl. Phys. 124, 086101 (2018)]. Journal of Applied Physics, 2018, 124, 086102.	2.5	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.	4.5	39
14	Efficient Computation of Sparse Matrix Functions for Large-Scale Electronic Structure Calculations: The <code>CheSS</code> Library. Journal of Chemical Theory and Computation, 2017, 13, 4684-4698.	5.3	23
15	Oxygen in silicon: Switch in the diffusion-mediated mechanism. Physical Review B, 2017, 96, .	3.2	2
16	Interface identification of the solid electrolyte interphase on graphite. Carbon, 2017, 111, 789-795.	10.3	15
17	Toward the III-V/Si co-integration by controlling the biatomic steps on hydrogenated Si(001). Applied Physics Letters, 2016, 109, .	3.3	46
18	Recent developments in the ABINIT software package. Computer Physics Communications, 2016, 205, 106-131.	7.5	662

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19	A wavelet-based Projector Augmented-Wave (PAW) method: Reaching frozen-core all-electron precision with a systematic, adaptive and localized wavelet basis set. <i>Computer Physics Communications</i> , 2016, 208, 1-8.	7.5	18
20	Reproducibility in density functional theory calculations of solids. <i>Science</i> , 2016, 351, aad3000.	12.6	1,113
21	An atomistic vision of the Mass Action Law: Prediction of carbon/oxygen defects in silicon. <i>Journal of Applied Physics</i> , 2015, 118, .	2.5	4
22	Accurate and efficient linear scaling DFT calculations with universal applicability. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 31360-31370.	2.8	158
23	Daubechies wavelets for linear scaling density functional theory. <i>Journal of Chemical Physics</i> , 2014, 140, 204110.	3.0	140
24	Lattice vacancies in silicon film exposed to external electric field. <i>Journal of Applied Physics</i> , 2013, 114, 043713.	2.5	3
25	Charge distribution and chemical bonding in B-O complexes in Cz-Si solar cells. <i>Journal of Applied Physics</i> , 2013, 114, 153708.	2.5	2
26	Impact of isovalent doping on the trapping of vacancy and interstitial related defects in Si. <i>Journal of Applied Physics</i> , 2013, 113, 113506.	2.5	61
27	Deciphering mechanisms of enhanced-retarded oxygen diffusion in doped Si. <i>Applied Physics Letters</i> , 2013, 103, .	3.3	9
28	Revisiting the domain model for lithium intercalated graphite. <i>Applied Physics Letters</i> , 2013, 103, .	3.3	33
29	Point defect diffusion in Si and SiGe revisited through atomistic simulations. <i>Materials Science in Semiconductor Processing</i> , 2012, 15, 675-690.	4.0	18
30	Crystal Structure of Cold Compressed Graphite. <i>Physical Review Letters</i> , 2012, 108, 065501.	7.8	292
31	Low-energy boron fullerenes: Role of disorder and potential synthesis pathways. <i>Physical Review B</i> , 2011, 83, .	3.2	37
32	Phase diagram, structure, and magnetic properties of the Ge-Mn system: A first-principles study. <i>Physical Review B</i> , 2011, 83, .	3.2	47
33	Vacancy-mediated diffusion in biaxially strained Si. <i>Applied Physics Letters</i> , 2011, 98, 031908.	3.3	11
34	Optimized energy landscape exploration using the <i>ab initio</i> based activation-relaxation technique. <i>Journal of Chemical Physics</i> , 2011, 135, 034102.	3.0	81
35	Correlation between Atomic Structure and Superglide of an Incommensurate Grain Boundary in Au. <i>Microscopy and Microanalysis</i> , 2010, 16, 1442-1443.	0.4	0
36	Structure of an incommensurate 90° Si grain boundary resolved with the help of a Cs-corrector for illumination. <i>Journal of Physics: Conference Series</i> , 2010, 209, 012041.	0.4	3

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37	First principles prediction of the metastability of the Ge ₂ Mn phase and its synthesis pathways. Applied Physics Letters, 2010, 96, 231904.	3.3	11
38	First-principles prediction of stable SiC cage structures and their synthesis pathways. Physical Review B, 2010, 82, .	3.2	37
39	Superglide at an Internal Incommensurate Boundary. Nano Letters, 2010, 10, 695-700.	9.1	23
40	ABINIT: First-principles approach to material and nanosystem properties. Computer Physics Communications, 2009, 180, 2582-2615.	7.5	2,297
41	Sharing electronic structure and crystallographic data with ETSF_IO. Computer Physics Communications, 2008, 179, 748-758.	7.5	9
42	Specification of an extensible and portable file format for electronic structure and crystallographic data. Computational Materials Science, 2008, 43, 1056-1065.	3.0	7
43	Daubechies wavelets as a basis set for density functional pseudopotential calculations. Journal of Chemical Physics, 2008, 129, 014109.	3.0	289
44	Germanium diffusion mechanisms in silicon from first principles. Physical Review B, 2007, 75, .	3.2	33
45	Vacancy-Assisted Diffusion in Silicon: A Three-Temperature-Regime Model. Physical Review Letters, 2006, 97, 135901.	7.8	44