

Audrius Alkauskas

List of Publications by Year in descending order

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72
papers

4,858
citations

101384

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91712

69
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96
all docs

96
docs citations

96
times ranked

5071
citing authors

#	ARTICLE	IF	CITATIONS
1	Tutorial: Defects in semiconductors – Combining experiment and theory. <i>Journal of Applied Physics</i> , 2016, 119, .	1.1	297
2	Defect Energy Levels in Density Functional Calculations: Alignment and Band Gap Problem. <i>Physical Review Letters</i> , 2008, 101, 046405.	2.9	263
3	First-principles theory of nonradiative carrier capture via multiphonon emission. <i>Physical Review B</i> , 2014, 90, .	1.1	263
4	Defect levels through hybrid density functionals: Insights and applications. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 775-789.	0.7	253
5	Band Offsets at Semiconductor-Oxide Interfaces from Hybrid Density-Functional Calculations. <i>Physical Review Letters</i> , 2008, 101, 106802.	2.9	229
6	Native point defects and impurities in hexagonal boron nitride. <i>Physical Review B</i> , 2018, 97, .	1.1	200
7	First-Principles Calculations of Luminescence Spectrum Line Shapes for Defects in Semiconductors: The Example of GaN and ZnO. <i>Physical Review Letters</i> , 2012, 109, 267401.	2.9	187
8	First-principles theory of the luminescence lineshape for the triplet transition in diamond NV centres. <i>New Journal of Physics</i> , 2014, 16, 073026.	1.2	183
9	Near-deterministic activation of room-temperature quantum emitters in hexagonal boron nitride. <i>Optica</i> , 2018, 5, 1128.	4.8	159
10	Measurement and Control of Single Nitrogen-Vacancy Center Spins above 600 ÅK. <i>Physical Review X</i> , 2012, 2, .	2.8	157
11	Optical Signatures of Quantum Emitters in Suspended Hexagonal Boron Nitride. <i>ACS Nano</i> , 2017, 11, 3328-3336.	7.3	150
12	Defect levels of dangling bonds in silicon and germanium through hybrid functionals. <i>Physical Review B</i> , 2008, 78, .	1.1	147
13	Band-edge problem in the theoretical determination of defect energy levels: The O vacancy in ZnO as a benchmark case. <i>Physical Review B</i> , 2011, 84, .	1.1	143
14	First-principles theory of acceptors in nitride semiconductors. <i>Physica Status Solidi (B): Basic Research</i> , 2015, 252, 900-908.	0.7	115
15	Hybrid-functional calculations with plane-wave basis sets: Effect of singularity correction on total energies, energy eigenvalues, and defect energy levels. <i>Physical Review B</i> , 2009, 80, .	1.1	112
16	Photoinduced Modification of Single-Photon Emitters in Hexagonal Boron Nitride. <i>ACS Photonics</i> , 2016, 3, 2490-2496.	3.2	109
17	A hybrid density functional study of lithium in ZnO: Stability, ionization levels, and diffusion. <i>Physical Review B</i> , 2009, 80, .	1.1	104
18	Observation of Individual Molecules Trapped on a Nanostructured Insulator. <i>Nano Letters</i> , 2004, 4, 2185-2189.	4.5	99

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19	First-Principles Calculations of Point Defects for Quantum Technologies. Annual Review of Materials Research, 2018, 48, 1-26.	4.3	93
20	Gallium vacancy complexes as a cause of Shockley-Read-Hall recombination in III-nitride light emitters. Applied Physics Letters, 2016, 108, .	1.5	91
21	Role of excited states in Shockley-Read-Hall recombination in wide-band-gap semiconductors. Physical Review B, 2016, 93, .	1.1	89
22	Charge transition levels of carbon-, oxygen-, and hydrogen-related defects at the SiC/SiO ₂ interface through hybrid functionals. Physical Review B, 2011, 84, .	1.1	86
23	Carbon dimer defect as a source of the 4.1 eV luminescence in hexagonal boron nitride. Applied Physics Letters, 2019, 115, .	1.5	77
24	Zn vacancy as a polaronic hole trap in ZnO. Physical Review B, 2017, 95, .	1.1	71
25	Dangling Bonds in Hexagonal Boron Nitride as Single-Photon Emitters. Physical Review Letters, 2019, 123, 127401.	2.9	68
26	Protecting a Diamond Quantum Memory by Charge State Control. Nano Letters, 2017, 17, 5931-5937.	4.5	66
27	Iron as a source of efficient Shockley-Read-Hall recombination in GaN. Applied Physics Letters, 2016, 109, .	1.5	64
28	Band alignments and defect levels in Si/HfO ₂ gate stacks: Oxygen vacancy and Fermi-level pinning. Applied Physics Letters, 2008, 92, .	1.5	63
29	Quantum defects by design. Nanophotonics, 2019, 8, 1867-1888.	2.9	58
30	Defect identification based on first-principles calculations for deep level transient spectroscopy. Applied Physics Letters, 2018, 113, .	1.5	51
31	Nonrad: Computing nonradiative capture coefficients from first principles. Computer Physics Communications, 2021, 267, 108056.	3.0	50
32	Defect levels of carbon-related defects at the SiC/SiO ₂ interface from hybrid functionals. Physical Review B, 2011, 83, .	1.1	45
33	First-principles study of the mobility of SrTiO ₃ . Physical Review B, 2014, 90, .	1.1	45
34	First principles investigation of defect energy levels at semiconductor-oxide interfaces: Oxygen vacancies and hydrogen interstitials in the Si/SiO ₂ /HfO ₂ stack. Journal of Applied Physics, 2009, 105, 061603.	1.1	41
35	Gaussian Form of Effective Core Potential and Response Function Basis Set Derived from Troullier-Martins Pseudopotential: Results for Ag and Au. Journal of Physical Chemistry A, 2004, 108, 6863-6868.	1.1	39
36	Zn vacancy-donor impurity complexes in ZnO. Physical Review B, 2018, 97, .	1.1	39

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37	Site-selective adsorption of naphthalene-tetracarboxylic-dianhydride on Ag(110): First-principles calculations. <i>Physical Review B</i> , 2006, 73, .	1.1	32
38	Dynamic structure factors of Cu, Ag, and Au: Comparative study from first principles. <i>Physical Review B</i> , 2013, 88, .	1.1	31
39	Electrical and optical properties of iron in GaN, AlN, and InN. <i>Physical Review B</i> , 2019, 99, .	1.1	30
40	Effect of improved band-gap description in density functional theory on defect energy levels in -quartz. <i>Physica B: Condensed Matter</i> , 2007, 401-402, 670-673.	1.3	29
41	Vibrational modes of negatively charged silicon-vacancy centers in diamond from <i>ab initio</i> calculations. <i>Physical Review B</i> , 2018, 98, .	1.1	27
42	Deep donor state of the copper acceptor as a source of green luminescence in ZnO. <i>Applied Physics Letters</i> , 2017, 111, 042101.	1.5	26
43	Alignment of hydrogen-related defect levels at the interface. <i>Physica B: Condensed Matter</i> , 2007, 401-402, 546-549.	1.3	25
44	Photoionization of negatively charged NV centers in diamond: Theory and <i>ab initio</i> calculations. <i>Physical Review B</i> , 2021, 104, .	1.1	25
45	Towards a Room-Temperature Spin Quantum Bus in Diamond via Electron Photoionization, Transport, and Capture. <i>Physical Review X</i> , 2016, 6, .	2.8	24
46	Vibrational and vibronic structure of isolated point defects: The nitrogen-vacancy center in diamond. <i>Physical Review B</i> , 2021, 104, .	1.1	24
47	Theoretical analysis of the momentum-dependent loss function of bulk Ag. <i>Ultramicroscopy</i> , 2010, 110, 1081-1086.	0.8	20
48	Calcium as a nonradiative recombination center in InGaN. <i>Applied Physics Express</i> , 2017, 10, 021001.	1.1	19
49	A hybrid functional scheme for defect levels and band alignments at semiconductor-oxide interfaces. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2010, 207, 270-276.	0.8	18
50	Spinning up quantum defects in 2D materials. <i>Nature Materials</i> , 2020, 19, 487-489.	13.3	18
51	Thermodynamics of carbon point defects in hexagonal boron nitride. <i>Physical Review Materials</i> , 2022, 6, .	0.9	17
52	Energy Level Alignment at Metal-Octaethylporphyrin Interfaces. <i>Journal of Physical Chemistry B</i> , 2005, 109, 23558-23563.	1.2	15
53	Charge state of the O_{Si} during silicon oxidation through hybrid functional calculations. <i>Physical Review B</i> , 2008, 78, .	1.1	15
54	Energy levels of candidate defects at SiC-SiO ₂ interfaces. <i>AIP Conference Proceedings</i> , 2010, , .	0.3	14

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55	Radiative capture rates at deep defects from electronic structure calculations. Physical Review B, 2020, 102, .	1.1	14
56	Strain broadening of the 1042-nm zero phonon line of the $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:msup} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{NV} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{no} \hat{\nu} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{center in diamond: A promising spectroscopic tool for defect tomography. Physical Review B, 2017, 96, .$	1.1	13
57	Negative- $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mi} \rangle \text{U} \langle \text{mml:mi} \rangle \langle \text{mml:math} \rangle$ and polaronic behavior of the Zn-O divacancy in ZnO. Physical Review B, 2019, 99, .	1.1	13
58	Deep-Level Defects and Impurities in InGaN Alloys. Physica Status Solidi (B): Basic Research, 2020, 257, 1900534.	0.7	13
59	Li-related defects in ZnO: Hybrid functional calculations. Physica B: Condensed Matter, 2009, 404, 4797-4799.	1.3	11
60	Comment on "Comparative study of <i>ab initio</i> nonradiative recombination rate calculations under different formalisms". Physical Review B, 2018, 97, .	1.1	11
61	Spin coherent quantum transport of electrons between defects in diamond. Nanophotonics, 2019, 8, 1975-1984.	2.9	11
62	Sign reversal of drag in bilayer systems with in-plane periodic potential modulation. Physical Review B, 2002, 66, .	1.1	7
63	Overcoming Bipolar Doping Difficulty in Wide Gap Semiconductors. , 2011, , 213-239.		7
64	Defects by design: Quantum nanophotonics in emerging materials. Nanophotonics, 2019, 8, 1863-1865.	2.9	6
65	Alignment of Defect Energy Levels at Si-SiO ₂ Interface from Hybrid Density Functional Calculations. , 2010, , .		5
66	Charge transition levels of the Ge dangling bond defect at Ge/insulator interfaces. Materials Science in Semiconductor Processing, 2008, 11, 226-229.	1.9	4
67	Capturing EELS in the reciprocal space. EPJ Applied Physics, 2011, 54, 33510.	0.3	3
68	Dynamics of Singlet Oxygen Molecule Trapped in Silica Glass Studied by Luminescence Polarization Anisotropy and Density Functional Theory. Journal of Physical Chemistry C, 2020, 124, 7244-7253.	1.5	3
69	Conformational stability of bicyclo[3.3.1]nonane-2,6-dione and bicyclo[3.3.1]nonane-2,9-dione: ab initio calculations and vibrational spectroscopy studies. Journal of Molecular Structure, 2001, 563-564, 517-521.	1.8	2
70	Advanced Calculations for Defects in Solids " Electronic Structure Methods. Physica Status Solidi (B): Basic Research, 2011, 248, 17-18.	0.7	2
71	Room-temperature quantum emitter arrays in hexagonal boron nitride. , 2017, , .		2
72	Defect Levels of the Ge Dangling Bond Defect. , 2010, , .		1