Audrius Alkauskas

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4420517/publications.pdf

Version: 2024-02-01

72 papers	4,858 citations	101543 36 h-index	91884 69 g-index
96 all docs	96 docs citations	96 times ranked	5071 citing authors

#	Article	IF	Citations
1	Tutorial: Defects in semiconductorsâ€"Combining experiment and theory. Journal of Applied Physics, 2016, 119, .	2.5	297
2	Defect Energy Levels in Density Functional Calculations: Alignment and Band Gap Problem. Physical Review Letters, 2008, 101, 046405.	7.8	263
3	First-principles theory of nonradiative carrier capture via multiphonon emission. Physical Review B, 2014, 90, .	3.2	263
4	Defect levels through hybrid density functionals: Insights and applications. Physica Status Solidi (B): Basic Research, 2011, 248, 775-789.	1.5	253
5	Band Offsets at Semiconductor-Oxide Interfaces from Hybrid Density-Functional Calculations. Physical Review Letters, 2008, 101, 106802.	7.8	229
6	Native point defects and impurities in hexagonal boron nitride. Physical Review B, 2018, 97, .	3.2	200
7	First-Principles Calculations of Luminescence Spectrum Line Shapes for Defects in Semiconductors: The Example of GaN and ZnO. Physical Review Letters, 2012, 109, 267401.	7.8	187
8	First-principles theory of the luminescence lineshape for the triplet transition in diamond NV centres. New Journal of Physics, 2014, 16, 073026.	2.9	183
9	Near-deterministic activation of room-temperature quantum emitters in hexagonal boron nitride. Optica, 2018, 5, 1128.	9.3	159
10	Measurement and Control of Single Nitrogen-Vacancy Center Spins above 600ÂK. Physical Review X, 2012, 2, .	8.9	157
11	Optical Signatures of Quantum Emitters in Suspended Hexagonal Boron Nitride. ACS Nano, 2017, 11, 3328-3336.	14.6	150
12	Defect levels of dangling bonds in silicon and germanium through hybrid functionals. Physical Review B, 2008, 78, .	3.2	147
13	Band-edge problem in the theoretical determination of defect energy levels: The O vacancy in ZnO as a benchmark case. Physical Review B, 2011, 84, .	3.2	143
14	Firstâ€principles theory of acceptors in nitride semiconductors. Physica Status Solidi (B): Basic Research, 2015, 252, 900-908.	1.5	115
15	Hybrid-functional calculations with plane-wave basis sets: Effect of singularity correction on total energies, energy eigenvalues, and defect energy levels. Physical Review B, 2009, 80, .	3.2	112
16	Photoinduced Modification of Single-Photon Emitters in Hexagonal Boron Nitride. ACS Photonics, 2016, 3, 2490-2496.	6.6	109
17	A hybrid density functional study of lithium in ZnO: Stability, ionization levels, and diffusion. Physical Review B, 2009, 80, .	3.2	104
18	Observation of Individual Molecules Trapped on a Nanostructured Insulator. Nano Letters, 2004, 4, 2185-2189.	9.1	99

#	Article	IF	Citations
19	First-Principles Calculations of Point Defects for Quantum Technologies. Annual Review of Materials Research, 2018, 48, 1-26.	9.3	93
20	Gallium vacancy complexes as a cause of Shockley-Read-Hall recombination in III-nitride light emitters. Applied Physics Letters, 2016, 108, .	3.3	91
21	Role of excited states in Shockley-Read-Hall recombination in wide-band-gap semiconductors. Physical Review B, 2016, 93, .	3.2	89
22	Charge transition levels of carbon-, oxygen-, and hydrogen-related defects at the SiC/SiO<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>interface through hybrid functionals. Physical Review B, 2011, 84, .	3.2	86
23	Carbon dimer defect as a source of the 4.1 eV luminescence in hexagonal boron nitride. Applied Physics Letters, 2019, 115, .	3.3	77
24	Zn vacancy as a polaronic hole trap in ZnO. Physical Review B, 2017, 95, .	3.2	71
25	Dangling Bonds in Hexagonal Boron Nitride as Single-Photon Emitters. Physical Review Letters, 2019, 123, 127401.	7.8	68
26	Protecting a Diamond Quantum Memory by Charge State Control. Nano Letters, 2017, 17, 5931-5937.	9.1	66
27	Iron as a source of efficient Shockley-Read-Hall recombination in GaN. Applied Physics Letters, 2016, 109, .	3.3	64
28	Band alignments and defect levels in Siâ€“HfO2 gate stacks: Oxygen vacancy and Fermi-level pinning. Applied Physics Letters, 2008, 92, .	3.3	63
29	Quantum defects by design. Nanophotonics, 2019, 8, 1867-1888.	6.0	58
30	Defect identification based on first-principles calculations for deep level transient spectroscopy. Applied Physics Letters, 2018, 113, .	3.3	51
31	Nonrad: Computing nonradiative capture coefficients from first principles. Computer Physics Communications, 2021, 267, 108056.	7.5	50
32	Defect levels of carbon-related defects at the SiC/SiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>interface from hybrid functionals. Physical Review B, 2011, 83, .	3.2	45
33	First-principles study of the mobility of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2014, 90, .	3.2	45
34	First principles investigation of defect energy levels at semiconductor-oxide interfaces: Oxygen vacancies and hydrogen interstitials in the Siâ€“SiO2â€“HfO2 stack. Journal of Applied Physics, 2009, 105, 061603.	2.5	41
35	Gaussian Form of Effective Core Potential and Response Function Basis Set Derived from Troullierâ'Martins Pseudopotential:â€‰ Results for Ag and Au. Journal of Physical Chemistry A, 2004, 108, 6863-6868.	2.5	39
36	Zn vacancy-donor impurity complexes in ZnO. Physical Review B, 2018, 97, .	3.2	39

#	Article	IF	Citations
37	Site-selective adsorption of naphthalene-tetracarboxylic-dianhydride onAg(110): First-principles calculations. Physical Review B, 2006, 73, .	3.2	32
38	Dynamic structure factors of Cu, Ag, and Au: Comparative study from first principles. Physical Review B, 2013, 88, .	3.2	31
39	Electrical and optical properties of iron in GaN, AlN, and InN. Physical Review B, 2019, 99, .	3.2	30
40	Effect of improved band-gap description in density functional theory on defect energy levels in -quartz. Physica B: Condensed Matter, 2007, 401-402, 670-673.	2.7	29
41	Vibrational modes of negatively charged silicon-vacancy centers in diamond from ab initio calculations. Physical Review B, 2018, 98, .	3.2	27
42	Deep donor state of the copper acceptor as a source of green luminescence in ZnO. Applied Physics Letters, 2017, 111, 042101.	3.3	26
43	Alignment of hydrogen-related defect levels at the interface. Physica B: Condensed Matter, 2007, 401-402, 546-549.	2.7	25
44	Photoionization of negatively charged NV centers in diamond: Theory and ab initio calculations. Physical Review B, 2021, 104, .	3.2	25
45	Towards a Room-Temperature Spin Quantum Bus in Diamond via Electron Photoionization, Transport, and Capture. Physical Review X, 2016, 6, .	8.9	24
46	Vibrational and vibronic structure of isolated point defects: The nitrogen-vacancy center in diamond. Physical Review B, 2021, 104, .	3.2	24
47	Theoretical analysis of the momentum-dependent loss function of bulk Ag. Ultramicroscopy, 2010, 110, 1081-1086.	1.9	20
48	Calcium as a nonradiative recombination center in InGaN. Applied Physics Express, 2017, 10, 021001.	2.4	19
49	A hybrid functional scheme for defect levels and band alignments at semiconductorâ€“oxide interfaces. Physica Status Solidi (A) Applications and Materials Science, 2010, 207, 270-276.	1.8	18
50	Spinning up quantum defects in 2D materials. Nature Materials, 2020, 19, 487-489.	27.5	18
51	Thermodynamics of carbon point defects in hexagonal boron nitride. Physical Review Materials, 2022, 6, .	2.4	17
52	Energy Level Alignment at Metalâˆ'Octaethylporphyrin Interfaces. Journal of Physical Chemistry B, 2005, 109, 23558-23563.	2.6	15
53	Charge state of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>O</mml:mtext><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:ma during silicon oxidation through hybrid functional calculations. Physical Review B, 2008, 78, .	3.2	15
54	Energy levels of candidate defects at SiCâˆ•SiO[sub 2] interfaces. AIP Conference Proceedings, 2010, , .	0.4	14

#	Article	IF	Citations
55	Radiative capture rates at deep defects from electronic structure calculations. Physical Review B, 2020, 102, .	3.2	14
56	Strain broadening of the 1042-nm zero phonon line of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mi>NV</mml:mi></mml:mrow><mml:mo>â˜’</m center in diamond: A promising spectroscopic tool for defect tomography. Physical Review B, 2017, 96, .	3.2	13
57	Negative-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>U</mml:mi></mml:math>and polaronic behavior of the Zn-O divacancy in ZnO. Physical Review B, 2019, 99, .	3.2	13
58	Deepâ€Level Defects and Impurities in InGaN Alloys. Physica Status Solidi (B): Basic Research, 2020, 257, 1900534.	1.5	13
59	Li-related defects in ZnO: Hybrid functional calculations. Physica B: Condensed Matter, 2009, 404, 4797-4799.	2.7	11
60	Comment on â€œComparative study of ab initio nonradiative recombination rate calculations under different formalismsâ€• Physical Review B, 2018, 97, .	3.2	11
61	Spin coherent quantum transport of electrons between defects in diamond. Nanophotonics, 2019, 8, 1975-1984.	6.0	11
62	Sign reversal of drag in bilayer systems with in-plane periodic potential modulation. Physical Review B, 2002, 66, .	3.2	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.	6.0	6
65	Alignment of Defect Energy Levels at Si-SiO[sub 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.	4.0	4
67	Capturing EELS in the reciprocal space. EPJ Applied Physics, 2011, 54, 33510.	0.7	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.	3.1	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.	3.6	2
70	Advanced Calculations for Defects in Solids â€“ Electronic Structure Methods. Physica Status Solidi (B): Basic Research, 2011, 248, 17-18.	1.5	2
71	Room-temperature quantum emitter arrays in hexagonal boron nitride. , 2017, , .		2
72	Defect Levels of the Ge Dangling Bond Defect. , 2010, , .		1