

Ben Hourahine

List of Publications by Year in descending order

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96
papers

3,669
citations

236833

25
h-index

133188

59
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99
all docs

99
docs citations

99
times ranked

4358
citing authors

#	ARTICLE	IF	CITATIONS
1	DFTB+, a Sparse Matrix-Based Implementation of the DFTB Method. Journal of Physical Chemistry A, 2007, 111, 5678-5684.	1.1	1,523
2	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. Journal of Chemical Physics, 2020, 152, 124101.	1.2	589
3	Hydrogen molecules in silicon located at interstitial sites and trapped in voids. Physical Review B, 1998, 57, R12666-R12669.	1.1	89
4	Critical impact of Ehrlich-Schwoebel barrier on GaN surface morphology during homoepitaxial growth. Journal of Crystal Growth, 2016, 433, 36-42.	0.7	61
5	Rare earth doped III-nitrides for optoelectronics. EPJ Applied Physics, 2006, 36, 91-103.	0.3	59
6	Rapid Nondestructive Analysis of Threading Dislocations in Wurtzite Materials Using the Scanning Electron Microscope. Physical Review Letters, 2012, 108, 135503.	2.9	56
7	Radiation-hard semiconductor detectors for SuperLHC. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2005, 541, 189-201.	0.7	55
8	Treatment of Collinear and Noncollinear Electron Spin within an Approximate Density Functional Based Method. Journal of Physical Chemistry A, 2007, 111, 5622-5629.	1.1	55
9	Self-Interaction and Strong Correlation in DFTB. Journal of Physical Chemistry A, 2007, 111, 5671-5677.	1.1	52
10	The Interaction of Hydrogen with Deep Level Defects in Silicon. Solid State Phenomena, 2000, 71, 173-248.	0.3	50
11	Geometrical Mie theory for resonances in nanoparticles of any shape. Optics Express, 2011, 19, 21432.	1.7	44
12	Identification of the hexavacancy in silicon with the B80 optical center. Physical Review B, 2000, 61, 12594-12597.	1.1	38
13	Electrical activity of carbon-hydrogen centers in Si. Physical Review B, 2002, 66, .	1.1	37
14	Electronic behavior of rare-earth dopants in AlN: A density-functional study. Physical Review B, 2005, 72, .	1.1	36
15	A Real-Time Time-Dependent Density Functional Tight-Binding Implementation for Semiclassical Excited State Electron Nuclear Dynamics and Pump-Probe Spectroscopy Simulations. Journal of Chemical Theory and Computation, 2020, 16, 4454-4469.	2.3	36
16	Plasmon modes in single gold nanodiscs. Optics Express, 2014, 22, 12189.	1.7	35
17	Recent advancements in the development of radiation hard semiconductor detectors for S-LHC. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2005, 552, 7-19.	0.7	33
18	Luminescence of Eu ions in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ the entire alloy composition range. Physical Review B, 2009, 80, .		

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19	Calculation of internal and scattered fields of axisymmetric nanoparticles at any point in space. <i>Journal of Optics</i> , 2009, 11, 054009.	1.5	30
20	Development of radiation tolerant semiconductor detectors for the Super-LHC. <i>Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment</i> , 2005, 546, 99-107.	0.7	29
21	Initial Steps toward Automating the Fitting of DFTBRep(r)â€. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5637-5641.	1.1	28
22	Coincident Electron Channeling and Cathodoluminescence Studies of Threading Dislocations in GaN. <i>Microscopy and Microanalysis</i> , 2014, 20, 55-60.	0.2	27
23	Theory of SERS enhancement: general discussion. <i>Faraday Discussions</i> , 2017, 205, 173-211.	1.6	27
24	ELSI â€” An open infrastructure for electronic structure solvers. <i>Computer Physics Communications</i> , 2020, 256, 107459.	3.0	27
25	p-type surface doping of diamond: a first-principles study. <i>Journal of Physics Condensed Matter</i> , 2001, 13, 8973-8978.	0.7	26
26	A theoretical study of erbium in GaN. <i>Physica B: Condensed Matter</i> , 2006, 376-377, 512-515.	1.3	25
27	Evidence for trapped by carbon impurities in silicon. <i>Physica B: Condensed Matter</i> , 2001, 308-310, 197-201.	1.3	23
28	Theoretical study of rare earth point defects in GaN. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2008, 5, 2358-2360.	0.8	23
29	Local Vibrational Modes of Weakly Bound O-H Complexes in Si. <i>Materials Science Forum</i> , 1997, 258-263, 391-398.	0.3	22
30	Local vibrational modes of two neighboring substitutional carbon atoms in silicon. <i>Physical Review B</i> , 2000, 62, 158-165.	1.1	21
31	Electron channelling contrast imaging for III-nitride thin film structures. <i>Materials Science in Semiconductor Processing</i> , 2016, 47, 44-50.	1.9	21
32	Efficient tight-binding approach for the study of strongly correlated systems. <i>Physical Review B</i> , 2007, 76, .	1.1	20
33	Infrared activity of hydrogen molecules trapped in Si. <i>Physical Review B</i> , 2003, 67, .	1.1	19
34	InterstitialH2in germanium by Raman scattering andab initio calculations. <i>Physical Review B</i> , 2005, 72, .	1.1	19
35	A theoretical study of O chemisorption on GaN (0001)/(0001 $\bar{1}$,) surfaces. <i>Solid State Communications</i> , 1998, 108, 953-958.	0.9	18
36	Imaging and identifying defects in nitride semiconductor thin films using a scanning electron microscope. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2012, 209, 424-426.	0.8	16

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37	Electron channeling contrast imaging studies of nonpolar nitrides using a scanning electron microscope. Applied Physics Letters, 2013, 102, .	1.5	16
38	Directional-dependent thickness and bending rigidity of phosphorene. Physical Review B, 2016, 94, .	1.1	16
39	An Efficient LDA+U Based Tight Binding Approach. Journal of Physical Chemistry A, 2007, 111, 5665-5670.	1.1	15
40	Combined infrared absorption and modeling study of a dicarbon-dihydrogen defect in silicon. Physical Review B, 2000, 62, 12859-12867.	1.1	14
41	Weakly bound carbon-hydrogen complex in silicon. Physical Review B, 2000, 61, 16659-16666.	1.1	14
42	Formation of Helices in Graphene Nanoribbons under Torsion. Journal of Physical Chemistry Letters, 2014, 5, 4083-4087.	2.1	14
43	Determining GaN Nanowire Polarity and its Influence on Light Emission in the Scanning Electron Microscope. Nano Letters, 2019, 19, 3863-3870.	4.5	14
44	A molecular radical model for hydrogen and muonium in graphite. Journal of Physics Condensed Matter, 2001, 13, 2169-2175.	0.7	13
45	Vibrational properties of elemental hydrogen centres in Si, Ge and dilute SiGe alloys. Journal of Physics Condensed Matter, 2005, 17, S2155-S2164.	0.7	13
46	Subgrain structure and dislocations in WC-Co hard metals revealed by electron channelling contrast imaging. International Journal of Refractory Metals and Hard Materials, 2020, 87, 105159.	1.7	13
47	Anomalous Shift of the 1075 cm ⁻¹ ; Oxygen-Hydrogen Defect in Silicon. Materials Science Forum, 1997, 258-263, 277-282.	0.3	12
48	Collapsed carbon nanotubes: From nano to mesoscale via density functional theory-based tight-binding objective molecular modeling. Carbon, 2019, 143, 786-792.	5.4	12
49	Glide dislocations in diamond: first-principles calculations of similarities with and differences from silicon and the effects of hydrogen. Journal of Physics Condensed Matter, 2002, 14, 12689-12696.	0.7	11
50	Energy-weighted dynamical scattering simulations of electron diffraction modalities in the scanning electron microscope. Ultramicroscopy, 2018, 187, 98-106.	0.8	11
51	Defect evolution and interplay in n-type InN. Applied Physics Letters, 2012, 100, 091907.	1.5	10
52	Coherent control of radiation patterns of nonlinear multiphoton processes in nanoparticles. Scientific Reports, 2015, 5, 12040.	1.6	10
53	Kikuchi pattern simulations of backscattered and transmitted electrons. Journal of Microscopy, 2021, 284, 157-184.	0.8	10
54	DFTB and lanthanides. Journal of Physics: Conference Series, 2010, 242, 012005.	0.3	9

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55	Optical control of scattering, absorption and lineshape in nanoparticles. <i>Optics Express</i> , 2013, 21, 20322.	1.7	9
56	Ewald summation on a helix: A route to self-consistent charge density-functional based tight-binding objective molecular dynamics. <i>Journal of Chemical Physics</i> , 2013, 139, 094110.	1.2	9
57	Scanning electron microscopy as a flexible technique for investigating the properties of UV-emitting nitride semiconductor thin films. <i>Photonics Research</i> , 2019, 7, B73.	3.4	9
58	Hydrogen molecules and platelets in germanium. <i>Physica B: Condensed Matter</i> , 2006, 376-377, 105-108.	1.3	8
59	The geometrical nature of optical resonances: from a sphere to fused dimer nanoparticles. <i>Measurement Science and Technology</i> , 2012, 23, 084002.	1.4	8
60	Self-interstitial hydrogen complexes in silicon. <i>Physical Review B</i> , 1999, 59, 15729-15732.	1.1	7
61	Germanium hydrogen pairs in silicon. <i>Journal of Physics Condensed Matter</i> , 2003, 15, S2803-S2807.	0.7	7
62	Dislocation contrast in electron channelling contrast images as projections of strain-like components. <i>Materials Today: Proceedings</i> , 2018, 5, 14652-14661.	0.9	7
63	Structural and luminescence imaging and characterisation of semiconductors in the scanning electron microscope. <i>Semiconductor Science and Technology</i> , 2020, 35, 054001.	1.0	7
64	Evaluation of E. M. Fields and Energy Transport in Metallic Nanoparticles with Near Field Excitation. <i>Physical Science International Journal</i> , 2014, 4, 565-575.	0.3	7
65	Coherent control of plasmons in nanoparticles with nonlocal response. <i>Optics Communications</i> , 2017, 382, 258-265.	1.0	6
66	Molecular hydrogen traps within silicon. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 1999, 58, 24-25.	1.7	5
67	Piezospectroscopic analysis of the hydrogen-carbon complexes in silicon. <i>Physica B: Condensed Matter</i> , 2001, 308-310, 139-142.	1.3	5
68	SITE MULTIPLICITY OF RARE EARTH IONS IN III-NITRIDES. <i>Materials Research Society Symposia Proceedings</i> , 2004, 831, 714.	0.1	5
69	Accurate light scattering for non spherical particles from Mie-type theory. <i>Journal of Physics: Conference Series</i> , 2012, 367, 012010.	0.3	5
70	Platinum and gold dihydrides in silicon. <i>Physica B: Condensed Matter</i> , 2003, 340-342, 668-672.	1.3	4
71	Characterization of the blue emission of Tm/Er co-implanted GaN. <i>Materials Research Society Symposia Proceedings</i> , 2005, 892, 544.	0.1	3
72	Luminescence spectroscopy of Eu-implanted zincblende GaN. <i>Physica Status Solidi (B): Basic Research</i> , 2008, 245, 170-173.	0.7	3

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73	Enhancing ultraviolet spontaneous emission with a designed quantum vacuum. Optics Express, 2017, 25, 4162.	1.7	3
74	Luminescence behavior of semipolar (10^{17} cm^{-3}) InGaN/GaN heterostructures on patterned Si substrates. Journal of Applied Physics, 2020, 127, 035705.	1.1	3
75	Optically active hydrogen dimers in silicon. Physica B: Condensed Matter, 1999, 273-274, 176-179.	1.3	2
76	Stable Hydrogen Pair Trapped at Carbon Impurities in Silicon. Defect and Diffusion Forum, 2003, 221-223, 1-10.	0.4	2
77	Hydrogen-related photoluminescent centers in SiC. Physical Review B, 2004, 70, .	1.1	2
78	Excited Multiplets of Eu in GaN. Materials Research Society Symposia Proceedings, 2011, 1290, 1.	0.1	2
79	Global search for stable screw dislocation cores in III-V semiconductors. Physica Status Solidi (A) Applications and Materials Science, 2012, 209, 71-74.	0.8	2
80	Simple models for InGaN alloys. Physica Status Solidi (A) Applications and Materials Science, 2012, 209, 79-82.	0.8	2
81	Applications of electron channeling contrast imaging for characterizing nitride semiconductor thin films. Microscopy and Microanalysis, 2012, 18, 684-685.	0.2	1
82	Dataset on coherent control of fields and induced currents in nonlinear multiphoton processes in a nanosphere. Scientific Data, 2015, 2, 150064.	2.4	1
83	Principal Modes of Maxwell's Equations. Springer Series on Atomic, Optical, and Plasma Physics, 2018, , 1-33.	0.1	1
84	Non-destructive imaging of residual strains in GaN and their effect on optical and electrical properties using correlative light-electron microscopy. Journal of Applied Physics, 2022, 131, 075303.	1.1	1
85	Structure and electrical activity of rare-earth dopants in selected III-Vs. Materials Research Society Symposia Proceedings, 2003, 798, 502.	0.1	0
86	CLEO ²⁰⁰⁹ /EUROPE-EQEC 2009 electromagnetic resonances in nanoparticles of arbitrary shape. , 2011, , .		0
87	Mode control of light scattering by nanoparticles. , 2013, , .		0
88	Strong near field coupling and enhanced energy extraction in metal nanostructures. , 2013, , .		0
89	Electron Channeling Contrast Imaging of Defects in III-Nitride Semiconductors. Microscopy and Microanalysis, 2014, 20, 1024-1025.	0.2	0
90	Reprint of: Electron channelling contrast imaging for III-nitride thin film structures. Materials Science in Semiconductor Processing, 2016, 55, 19-25.	1.9	0

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91	Non-destructive Imaging of Extend Defects in III-nitride Thin film Structures Using Electron Channelling Contrast Imaging. Microscopy and Microanalysis, 2017, 23, 570-571.	0.2	0
92	Dynamical Simulations of Transmission Kikuchi Diffraction (TKD) Patterns. Microscopy and Microanalysis, 2017, 23, 540-541.	0.2	0
93	Imaging Extended Defects in Low Z materials using Electron Channelling Contrast Imaging “ New Approaches and Challenges. Microscopy and Microanalysis, 2019, 25, 1760-1761.	0.2	0
94	Two beam toy model for dislocation contrast in ECCI. Microscopy and Microanalysis, 2019, 25, 1968-1969.	0.2	0
95	Advances in electron channelling contrast imaging and electron backscatter diffraction for imaging and analysis of structural defects in the scanning electron microscope. IOP Conference Series: Materials Science and Engineering, 2020, 891, 012023.	0.3	0
96	Ab Initio Studies of Hydrogen Molecules in Silicon. , 1999, , 155-163.		0