

Gabriel Bester

List of Publications by Year in descending order

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128
papers

4,808
citations

94433

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102487

66
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128
all docs

128
docs citations

128
times ranked

3887
citing authors

#	ARTICLE	IF	CITATIONS
1	The mechanism of proton conduction in phosphoric acid. <i>Nature Chemistry</i> , 2012, 4, 461-466.	13.6	428
2	Pseudopotential calculation of the excitonic fine structure of million-atom self-assembled $\text{In}_{1-x}\text{Ga}_x\text{As}/\text{GaAs}$ quantum dots. <i>Physical Review B</i> , 2003, 67, .	3.2	316
3	Theoretical and experimental examination of the intermediate-band concept for strain-balanced $(\text{In,Ga})\text{As}/\text{Ga}(\text{As,P})$ quantum dot solar cells. <i>Physical Review B</i> , 2008, 78, .	3.2	215
4	Cylindrically shaped zinc-blende semiconductor quantum dots do not have cylindrical symmetry: Atomistic symmetry, atomic relaxation, and piezoelectric effects. <i>Physical Review B</i> , 2005, 71, .	3.2	203
5	Importance of Second-Order Piezoelectric Effects in Zinc-Blende Semiconductors. <i>Physical Review Letters</i> , 2006, 96, 187602.	7.8	197
6	Nanowire Quantum Dots as an Ideal Source of Entangled Photon Pairs. <i>Physical Review Letters</i> , 2009, 103, 063601.	7.8	184
7	Tuning the Exciton Binding Energies in Single Self-Assembled InGaAs Quantum Dots by Piezoelectric-Induced Biaxial Stress. <i>Physical Review Letters</i> , 2010, 104, 067405.	7.8	160
8	Effects of linear and nonlinear piezoelectricity on the electronic properties of InAs/GaAs quantum dots. <i>Physical Review B</i> , 2006, 74, .	3.2	135
9	A light-hole exciton in a quantum dot. <i>Nature Physics</i> , 2014, 10, 46-51.	16.7	111
10	Peculiar many-body effects revealed in the spectroscopy of highly charged quantum dots. <i>Nature Physics</i> , 2007, 3, 774-779.	16.7	96
11	Excitons, biexcitons, and trions in self-assembled $(\text{In,Ga})\text{As}/\text{GaAs}$ quantum dots: Recombination energies, polarization, and radiative lifetimes versus dot height. <i>Physical Review B</i> , 2005, 72, .	3.2	93
12	Lower Bound for the Excitonic Fine Structure Splitting in Self-Assembled Quantum Dots. <i>Physical Review Letters</i> , 2010, 104, 196803.	7.8	88
13	Theory of Excitonic Spectra and Entanglement Engineering in Dot Molecules. <i>Physical Review Letters</i> , 2004, 93, 047401.	7.8	85
14	Conventional Optics from Unconventional Electronics in ZnO Quantum Dots. <i>Journal of Physical Chemistry C</i> , 2010, 114, 9301-9307.	3.1	81
15	Electronic excitations in nanostructures: an empirical pseudopotential based approach. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 023202.	1.8	79
16	Carrier relaxation mechanisms in self-assembled $(\text{In,Ga})\text{As}/\text{GaAs}$ quantum dots: Efficient Auger relaxation of electrons. <i>Physical Review B</i> , 2006, 74, .	3.2	71
17	Fine Structure of Negatively and Positively Charged Excitons in Semiconductor Quantum Dots: Electron-Hole Asymmetry. <i>Physical Review Letters</i> , 2007, 98, 036808.	7.8	70
18	Broken symmetry and quantum entanglement of an exciton in $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ quantum dot molecules. <i>Physical Review B</i> , 2005, 71, .	3.2	69

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19	Interpretation of ab initio total energy results in a chemical language: I. Formalism and implementation into a mixed-basis pseudopotential code. <i>Journal of Physics Condensed Matter</i> , 2001, 13, 11541-11550.	1.8	65
20	First- and second-order piezoelectricity in III-V semiconductors. <i>Physical Review B</i> , 2011, 84, .	3.2	65
21	Nonlinear piezoelectricity in wurtzite semiconductors. <i>Physical Review B</i> , 2013, 88, .	3.2	61
22	Electronic and optical properties of ZnO quantum dots under hydrostatic pressure. <i>Physical Review B</i> , 2013, 87, .	3.2	54
23	Hydrofluorinated graphene: Two-dimensional analog of polyvinylidene fluoride. <i>Physical Review B</i> , 2011, 84, .	3.2	48
24	Compositional and size-dependent spectroscopic shifts in charged self-assembled $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ quantum dots. <i>Physical Review B</i> , 2003, 68, .	3.2	47
25	Full-Zone Spin Splitting for Electrons and Holes in Bulk GaAs and GaSb. <i>Physical Review Letters</i> , 2009, 102, 056405.	7.8	47
26	Strain-induced interfacial hole localization in self-assembled quantum dots: $\text{Compressive InAs/GaAs}$ versus tensile InAs/Sb . <i>Physical Review B</i> , 2004, 70, .	3.2	45
27	Structure of quantum dots as seen by excitonic spectroscopy versus structural characterization: Using theory to close the loop. <i>Physical Review B</i> , 2009, 80, .	3.2	45
28	Transition in the Optical Emission Polarization of ZnO Nanorods. <i>Journal of Physical Chemistry C</i> , 2011, 115, 15862-15867.	3.1	44
29	Dependence of the electronic structure of self-assembled $(\text{In,Ga})\text{As/GaAs}$ quantum dots on height and composition. <i>Journal of Applied Physics</i> , 2005, 98, 043708.	2.5	43
30	First principles molecular dynamics study of proton dynamics and transport in phosphoric acid/imidazole (2:1) system. <i>Solid State Ionics</i> , 2013, 252, 34-39.	2.7	43
31	Effective formation energies of atomic defects in $\text{D}_{03\bar{1}}\text{-Fe}_3\text{Al}$: an ab-initio study. <i>Intermetallics</i> , 1997, 5, 597-600.	3.9	42
32	Experimental imaging and atomistic modeling of electron and hole quasiparticle wave functions in InAs/GaAs quantum dots. <i>Physical Review B</i> , 2007, 75, 041405.	3.2	42
33	Prediction of a Shape-Induced Enhancement in the Hole Relaxation in Nanocrystals. <i>Nano Letters</i> , 2003, 3, 1197-1202.	9.1	41
34	Excitonic exchange effects on the radiative decay time of monoexcitons and biexcitons in quantum dots. <i>Physical Review B</i> , 2006, 74, .	3.2	41
35	Discovery of a Novel Linear-in- k Spin Splitting for Holes in the 2D GaAs/AlAs System. <i>Physical Review Letters</i> , 2010, 104, 066405.	7.8	41
36	Dependence of the Redshifted and Blueshifted Photoluminescence Spectra of Single $\text{In}_x\text{Ga}_{1-x}$ Dots on the Applied Uniaxial Stress. <i>Physical Review Letters</i> , 2011, 107, 217402.	7.8	40

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37	Singlet-triplet splitting, correlation, and entanglement of two electrons in quantum dot molecules. <i>Physical Review B</i> , 2005, 72, .	3.2	37
38	Controlling quantum dot emission by integration of semiconductor nanomembranes onto piezoelectric actuators. <i>Physica Status Solidi (B): Basic Research</i> , 2012, 249, 687-696.	1.5	36
39	Uniaxial stress flips the natural quantization axis of a quantum dot for integrated quantum photonics. <i>Nature Communications</i> , 2018, 9, 3058.	12.8	35
40	Confinement effects on the vibrational properties of III-V and II-VI nanoclusters. <i>Physical Review B</i> , 2012, 85, .	3.2	34
41	Electric field control and optical signature of entanglement in quantum dot molecules. <i>Physical Review B</i> , 2005, 72, .	3.2	33
42	Atomic defects in the ordered compound B ₂ -CoAl: A combination of ab initio electron theory and statistical mechanics. <i>Physical Review B</i> , 1999, 60, 14492-14495.	3.2	31
43	Analysis of the electronic structure of intermetallic compounds, and application to structural defects in B ₂ phases. <i>Journal of Alloys and Compounds</i> , 2000, 308, 1-14.	5.5	31
44	Electronic Phase Diagrams of Carriers in Self-Assembled Quantum Dots: Violation of Hund's Rule and the Aufbau Principle for Holes. <i>Physical Review Letters</i> , 2005, 95, 246804.	7.8	31
45	Supercoupling between heavy-hole and light-hole states in nanostructures. <i>Physical Review B</i> , 2015, 92, .	3.2	31
46	First-principles calculation of the electron-phonon interaction in semiconductor nanoclusters. <i>Physical Review B</i> , 2012, 85, .	3.2	30
47	Large nuclear zero-point motion effect in semiconductor nanoclusters. <i>Physical Review B</i> , 2013, 88, .	3.2	28
48	Prediction of an Excitonic Ground State in InAs/InSb Quantum Dots. <i>Physical Review Letters</i> , 2005, 94, 016801.	7.8	26
49	Mechanism of Efficient Proton Conduction in Diphosphoric Acid Elucidated via First-Principles Simulation and NMR. <i>Journal of Physical Chemistry B</i> , 2015, 119, 15866-15875.	2.6	26
50	Charged excitons and biexcitons in laterally coupled (In,Ga)As quantum dots. <i>Physical Review B</i> , 2010, 82, .	3.2	25
51	Heterogeneous confinement in laterally coupled InGaAs/GaAs quantum dot molecules under lateral electric fields. <i>Physical Review B</i> , 2010, 81, .	3.2	25
52	Artificial Atoms in Magnetic Fields: Wave-Function Shaping and Phase-Sensitive Tunneling. <i>Physical Review Letters</i> , 2010, 105, 176804.	7.8	25
53	Atomistic pseudopotential calculations of thickness-fluctuation GaAs quantum dots. <i>Physical Review B</i> , 2009, 79, .	3.2	24
54	Interatomic potentials for the vibrational properties of III-V semiconductor nanostructures. <i>Physical Review B</i> , 2011, 83, .	3.2	24

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55	Carrier relaxation in colloidal nanocrystals: Bridging large electronic energy gaps by low-energy vibrations. <i>Physical Review B</i> , 2015, 91, .	3.2	23
56	Electronic asymmetry in self-assembled quantum dot molecules made of identical InAs/GaAs quantum dots. <i>Physical Review B</i> , 2005, 72, .	3.2	22
57	From Wurtzite Nanoplatelets to Zinc Blende Nanorods: Simultaneous Control of Shape and Phase in Ultrathin ZnS Nanocrystals. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3828-3835.	4.6	21
58	First-principles many-body theory for charged and neutral excitations: Trion fine structure splitting in transition metal dichalcogenides. <i>Physical Review B</i> , 2019, 100, .	3.2	21
59	Photoluminescence of Fully Inorganic Colloidal Gold Nanocluster and Their Manipulation Using Surface Charge Effects. <i>Advanced Materials</i> , 2021, 33, e2101549.	21.0	21
60	Coexistence and coupling of zero-dimensional, two-dimensional, and continuum resonances in nanostructures. <i>Physical Review B</i> , 2009, 80, .	3.2	20
61	Strain-induced localized states within the matrix continuum of self-assembled quantum dots. <i>Applied Physics Letters</i> , 2009, 95, 023108.	3.3	20
62	Effects of atomic ordering on the electronic and optical properties of self-assembled In _x Ga _{1-x} semiconductor quantum dots. <i>Physical Review B</i> , 2011, 84, .	3.2	20
63	Interpretation of ab initio total energy results in a chemical language: II. Stability of TiAl ₃ and ScAl ₃ . <i>Journal of Physics Condensed Matter</i> , 2001, 13, 11551-11565.	1.8	19
64	Confinement-Induced versus Correlation-Induced Electron Localization and Wave Function Entanglement in Semiconductor Nano Dumbbells. <i>Nano Letters</i> , 2006, 6, 1069-1074.	9.1	19
65	Long- and short-range electron-hole exchange interaction in different types of quantum dots. <i>New Journal of Physics</i> , 2009, 11, 123024.	2.9	19
66	Atomic defects in D ₀₃ -Ni ₃ Sb: An ab initio study. <i>Physical Review B</i> , 1998, 57, R11019-R11022.	3.2	18
67	Comment on "Point defect behavior in high temperature region in the B2-type intermetallic compound FeAl" by M. Kogachi, T. Haraguchi and S.M. Kim. <i>Intermetallics</i> , 1999, 7, 1307-1308.	3.9	17
68	Structural vacancies in B2 CoAl and NiAl. <i>Scripta Materialia</i> , 2001, 44, 2485-2488.	5.2	17
69	Pressure effects on neutral and charged excitons in self-assembled (In,Ga)As/GaAs quantum dots. <i>Physical Review B</i> , 2005, 72, .	3.2	17
70	Influence of the atomic-scale structure on the exciton fine-structure splitting in InGaAs and GaAs quantum dots in a vertical electric field. <i>Physical Review B</i> , 2012, 86, .	3.2	17
71	Heavy strain conditions in colloidal core-shell quantum dots and their consequences on the vibrational properties from <i>ab initio</i> calculations. <i>Physical Review B</i> , 2015, 92, .	3.2	17
72	Direct Quantitative Electrical Measurement of Many-Body Interactions in Exciton Complexes in InAs Quantum Dots. <i>Physical Review Letters</i> , 2014, 112, 046803.	7.8	16

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73	Diffusion in Metals and Intermetallic Compounds: The Impact of AB-INITIO Calculations. Materials Research Society Symposia Proceedings, 1998, 527, 23.	0.1	15
74	Influence of the charge carrier tunneling processes on the recombination dynamics in single lateral quantum dot molecules. Physical Review B, 2010, 82, .	3.2	15
75	Atomic effective pseudopotentials for semiconductors. Physical Review B, 2012, 86, .	3.2	15
76	Dominant thermal defects in B ₂ FeAl. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2002, 323, 487-490.	5.6	14
77	Near-band-edge exciton polarization change in ZnO nanowires. Physical Chemistry Chemical Physics, 2015, 17, 1197-1203.	2.8	14
78	Semiempirical pseudopotential approach for nitride-based nanostructures and <i>ab initio</i> -based passivation of free surfaces. Physical Review B, 2012, 86, .	3.2	13
79	Surface-bound states in nanodiamonds. Physical Review B, 2017, 95, .	3.2	13
80	Realization of linearly polarized exciton emission in wurtzite zinc oxide quantum dots. Physical Review B, 2018, 98, .	3.2	13
81	Dielectric response function for colloidal semiconductor quantum dots. Journal of Chemical Physics, 2019, 151, 224103.	3.0	13
82	On the meaning of effective formation entropies for atomic defects in ordered compounds. Scripta Materialia, 1998, 39, 1071-1075.	5.2	12
83	Interlayer contraction in MgB ₂ upon replacement of Mg by Al: Effect of the covalent bond energy. Physical Review B, 2005, 72, .	3.2	12
84	Thermodynamics and nonstoichiometry in the D0 ₃ compound Ni ₃ Sb. Intermetallics, 2007, 15, 862-868.	3.9	12
85	Insights about the Surface of Colloidal Nanoclusters from Their Vibrational and Thermodynamic Properties. Journal of Physical Chemistry C, 2012, 116, 10790-10795.	3.1	12
86	Band gap renormalization of diamondoids: vibrational coupling and excitonic effects. New Journal of Physics, 2016, 18, 113052.	2.9	12
87	Excitonic optical properties of wurtzite ZnS quantum dots under pressure. Journal of Chemical Physics, 2015, 142, 114305.	3.0	11
88	Tuning of the Optical Emission Polarization of ZnO Nanorods by an Applied Hydrostatic Pressure. Journal of Physical Chemistry C, 2012, 116, 26592-26597.	3.1	10
89	Effects of charged defects on the electronic and optical properties of self-assembled quantum dots. Physical Review B, 2012, 85, .	3.2	9
90	Large-scale atomic effective pseudopotential program including an efficient spin-orbit coupling treatment in real space. Physical Review B, 2015, 91, .	3.2	9

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91	Fundamental difference between measured and calculated exciton-phonon coupling in nanostructures. <i>Physical Review B</i> , 2019, 99, .	3.2	9
92	Excitonic fine structure of zinc-blende and wurtzite colloidal CdSe nanocrystals and comparison to effective mass results. <i>Physical Review B</i> , 2020, 101, .	3.2	9
93	Excitons in ZnO Quantum Dots: The Role of Dielectric Confinement. <i>Journal of Physical Chemistry C</i> , 2022, 126, 2833-2838.	3.1	9
94	Theoretical predictions of the electronic and optical properties of single and coupled (In,Ga)As/GaAs quantum dots. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2006, 32, 93-96.	2.7	8
95	Force field potentials for the vibrational properties of II-VI semiconductor nanostructures. <i>Physical Review B</i> , 2017, 96, .	3.2	8
96	Optical properties of zig-zag and armchair ZnO colloidal nanoribbons. <i>Chemical Physics Letters</i> , 2019, 732, 136659.	2.6	8
97	Role of Magnetic Coupling in Photoluminescence Kinetics of Mn ²⁺ -Doped ZnS Nanoplatelets. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 18806-18815.	8.0	8
98	Predicting the electronic properties of 3D, million-atom semiconductor nanostructure architectures. <i>Journal of Physics: Conference Series</i> , 2006, 46, 292-298.	0.4	7
99	Excitonic fine structure, charged exciton, and multiexciton wave functions in self-assembled In _x As _{1-x} Ga _{1-x} quantum dots. <i>Physical Review B</i> , 2007, 75, 045307.	3.2	7
100	Quantum-dot intermediate-band solar cells with inverted band alignment. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2008, 41, 15-17.	2.7	7
101	Exciton-Related Raman Scattering, Interband Absorption and Photoluminescence in Colloidal CdSe/CdS Core/Shell Quantum Dots Ensemble. <i>Nanomaterials</i> , 2021, 11, 1274.	4.1	7
102	Theory of excitons, charged excitons, exciton fine-structure and entangled excitons in self-assembled semiconductor quantum dots. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2004, 21, 204-210.	2.7	6
103	Excitonic fine structure and optical properties of strained In _x As _{1-x} Ga _{1-x} quantum dots. <i>Physical Review B</i> , 2007, 75, 045307.	3.2	6
104	Intraband dynamics of mid-infrared HgTe quantum dots. <i>Nanoscale</i> , 2022, 14, 4123-4130.	5.6	6
105	Publisher's Note: Singlet-triplet splitting, correlation, and entanglement of two electrons in quantum dot molecules [Phys. Rev. B72, 195307 (2005)]. <i>Physical Review B</i> , 2005, 72, .	3.2	5
106	A thermodynamic study of the D03-ordered intermetallic compound Fe ₃ Al. <i>Journal of Alloys and Compounds</i> , 2008, 458, 277-281.	5.5	5
107	Vibron-phonon coupling from ab initio molecular dynamics simulations of a silicon cluster. <i>New Journal of Physics</i> , 2013, 15, 043039.	2.9	5
108	Nonspherical atomic effective pseudopotentials for surface passivation. <i>Physical Review B</i> , 2016, 94, .	3.2	5

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109	Biexcitons fine structure and non-equilibrium effects in transition metal dichalcogenides monolayers from first principles. <i>Communications Physics</i> , 2021, 4, .	5.3	5
110	Screened configuration interaction method for open-shell excited states applied to NV centers. <i>Physical Review B</i> , 2021, 104, .	3.2	5
111	Single Crystalline Colloidal Quasi-2D Tin Telluride. <i>Advanced Materials Interfaces</i> , 2020, 7, 2000410.	3.7	5
112	Ab initio calculation of the activation energy for Ni self-diffusion in D03 Ni3Sb. <i>Physical Review B</i> , 1999, 59, 3274-3275.	3.2	4
113	On the electronic structure of the pure and oxygen covered Ru() surface. <i>Surface Science</i> , 2002, 497, 305-310.	1.9	4
114	Morphology control of exciton fine structure in polar and nonpolar zinc sulfide nanorods. <i>Scientific Reports</i> , 2017, 7, 9366.	3.3	4
115	Phonon-Assisted Auger Process Enables Ultrafast Charge Transfer in CdSe Quantum Dot/Organic Molecule. <i>Journal of Physical Chemistry C</i> , 2019, 123, 17127-17135.	3.1	4
116	Effect of IT-M doping on charge transfer and ultrafast carrier dynamics of ternary organic solar cell materials. <i>Journal Physics D: Applied Physics</i> , 2020, 53, 095103.	2.8	4
117	NanoPSE: Nanoscience Problem Solving Environment for atomistic electronic structure of semiconductor nanostructures. <i>Journal of Physics: Conference Series</i> , 2005, 16, 277-282.	0.4	3
118	Manipulating fine structure splitting in semiconductor quantum dots. <i>Journal of Physics: Conference Series</i> , 2010, 245, 012008.	0.4	3
119	Exchange Spin Coupling in Optically Excited States. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4708-4718.	5.3	3
120	Publisher's Note: Broken symmetry and quantum entanglement of an exciton in In _x Ga _{1-x} As quantum dot molecules [Phys. Rev. B71, 075325 (2005)]. <i>Physical Review B</i> , 2005, 71, .	3.2	1
121	Growth and spectroscopy of single lateral InGaAs/GaAs quantum dot molecules. <i>Physica Status Solidi (B): Basic Research</i> , 2012, 249, 710-720.	1.5	1
122	Ab-Initio Calculations of the Vibrational Properties and Dynamical Processes in Semiconductor Nanostructures. , 2016, , 171-186.		1
123	Atomistic Pseudopotential Theory of Droplet Epitaxial GaAs/AlGaAs Quantum Dots. <i>Lecture Notes in Nanoscale Science and Technology</i> , 2013, , 329-361.	0.8	1
124	From the Electronic Structure to the Macroscopic Behavior: A Multi-scale Analysis of Plasticity in Intermetallic Compounds. <i>Materials Research Society Symposia Proceedings</i> , 2000, 652, 1.	0.1	0
125	Hydro-, Chloro- and Fluorographene Structures: A Density Functional Based Study. , 2011, , .		0
126	Ab-Initio Calculations of the Vibrational Properties of Nanostructures. , 2013, , 145-156.		0

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127	Ab-Initio Calculations of the Vibrational Properties of Nanostructures. , 2013, , 167-181.		0
128	Ultrafast DC-Stark shifting of a single quantum dot. , 2013, , .		0