Adam Gali

List of Publications by Year
in descending order

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313 papers	13,065 citations	22099 59 h-index	32761 100 g-index
329 all docs	329 docs citations	329 times ranked	7825 citing authors

#	Article	IF	Citations
1	Room-temperature coherent manipulation of single-spin qubits in silicon carbide with a high readout contrast. National Science Review, 2022, 9, .	4.6	44
2	Ultrahigh nitrogen-vacancy center concentration in diamond. Carbon, 2022, 188, 393-400.	5.4	9
3	Photoluminescence spectrum of divacancy in porous and nanocrystalline cubic silicon carbide. Journal of Applied Physics, 2022, 131, .	1.1	8
4	Carbon defect qubit in two-dimensional WS2. Nature Communications, 2022, 13, 1210.	5.8	12
5	Fluorescence spectrum and charge state control of divacancy qubits via illumination at elevated temperatures in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>4</mml:mn><mml:mi>H</mml:mi></mml:mrow></mml silicon carbide. Physical Review B, 2022, 105, .	1.1	5
6	Ultraviolet Quantum Emitters in Hexagonal Boron Nitride from Carbon Clusters. Journal of Physical Chemistry Letters, 2022, 13, 3150-3157.	2.1	11
7	Detection of Single W-Centers in Silicon. ACS Photonics, 2022, 9, 2337-2345.	3.2	29
8	Optimization of Chromium-Doped Zinc Gallate Nanocrystals for Strong Near-Infrared Emission by Annealing. ACS Applied Nano Materials, 2022, 5, 8950-8961.	2.4	5
9	Fundaments of photoelectric readout of spin states in diamond. Semiconductors and Semimetals, 2021, , 105-147.	0.4	2
10	Solar Photoelectroreduction of Nitrate Ions on PbI 2 /CuI Nanocomposite Electrodes. Solar Rrl, 2021, 5, 2000418.	3.1	4
11	Photoluminescence at the ground-state level anticrossing of the nitrogen-vacancy center in diamond: A comprehensive study. Physical Review B, 2021, 103, .	1.1	16
12	Enhancement of X-ray-Excited Red Luminescence of Chromium-Doped Zinc Gallate via Ultrasmall Silicon Carbide Nanocrystals. Chemistry of Materials, 2021, 33, 2457-2465.	3.2	9
13	Quantum guidelines for solid-state spin defects. Nature Reviews Materials, 2021, 6, 906-925.	23.3	185
14	Robust coherent control of solid-state spin qubits using anti-Stokes excitation. Nature Communications, 2021, 12, 3223.	5.8	19
15	Single-spin resonance in a van der Waals embedded paramagnetic defect. Nature Materials, 2021, 20, 1079-1084.	13.3	95
16	Highly tunable magneto-optical response from magnesium-vacancy color centers in diamond. Npj Quantum Information, 2021, 7, .	2.8	12
17	Room-temperature control and electrical readout of individual nitrogen-vacancy nuclear spins. Nature Communications, 2021, 12, 4421.	5.8	20
18	Towards identification of silicon vacancy-related electron paramagnetic resonance centers in 4H -SiC. Physical Review B, 2021, 104, .	1.1	9

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19	Towards ab initio identification of paramagnetic substitutional carbon defects in hexagonal boron nitride acting as quantum bits. Physical Review B, 2021, 104, .	1.1	48
20	DMRG on Top of Plane-Wave Kohnâ€“Sham Orbitals: A Case Study of Defected Boron Nitride. Journal of Chemical Theory and Computation, 2021, 17, 1143-1154.	2.3	16
21	Structure and Properties of Heavily B and P Codoped Amorphous Silicon Quantum Dots. Journal of Physical Chemistry C, 2021, 125, 23267-23274.	1.5	1
22	Strong Zero-Phonon Transition from Point Defect-Stacking Fault Complexes in Silicon Carbide Nanowires. Nano Letters, 2021, 21, 9187-9194.	4.5	7
23	Identification of a Telecom Wavelength Single Photon Emitter in Silicon. Physical Review Letters, 2021, 127, 196402.	2.9	22
24	Magneto-optical spectra of the split nickel-vacancy defect in diamond. Physical Review Research, 2021, 3, .	1.3	10
25	Spectroscopic investigations of negatively charged tin-vacancy centres in diamond. New Journal of Physics, 2020, 22, 013048.	1.2	62
26	Giant shift upon strain on the fluorescence spectrum of VNNB color centers in h-BN. Npj Quantum Information, 2020, 6, .	2.8	25
27	Material platforms for defect qubits and single-photon emitters. Applied Physics Reviews, 2020, 7, .	5.5	96
28	Stoneâ€“Wales defects in hexagonal boron nitride as ultraviolet emitters. Npj Computational Materials, 2020, 6, .	3.5	24
29	Ab initio determination of pseudospin for paramagnetic defects in SiC. Physical Review B, 2020, 102, .	1.1	10
30	Optically Detected Magnetic Resonance in Neutral Silicon Vacancy Centers in Diamond via Bound Exciton States. Physical Review Letters, 2020, 125, 237402.	2.9	36
31	Silicon-Carbide (SiC) Nanocrystal Technology and Characterization and Its Applications in Memory Structures. Nanomaterials, 2020, 10, 2387.	1.9	8
32	Ab initio theory of the negatively charged boron vacancy qubit in hexagonal boron nitride. Npj Computational Materials, 2020, 6, .	3.5	118
33	Vibronic States and Their Effect on the Temperature and Strain Dependence of Silicon-Vacancy Qubits in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mn>4</mml:mn><mml:mi>H</mml:mi></mml:math>-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mrow><mml:mi>Si</mml:mi><mml:mi mathvariant="normal">C</mml:mi></mml:mrow></mml:math>. Physical Review Applied, 2020, 13, .	1.5	47
34	Interlayer Bonding in Two-Dimensional Materials: The Special Case of SnP₃ and GeP₃. Journal of Physical Chemistry Letters, 2020, 11, 4503-4510.	2.1	24
35	Spin-controlled generation of indistinguishable and distinguishable photons from silicon vacancy centres in silicon carbide. Nature Communications, 2020, 11, 2516.	5.8	56
36	Room-temperature coherent control of implanted defect spins in silicon carbide. Npj Quantum Information, 2020, 6, .	2.8	25

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37	Novel Method for Electroless Etching of 6Hâ€“SiC. Nanomaterials, 2020, 10, 538.	1.9	6
38	Room-Temperature Defect Qubits in Ultrasmall Nanocrystals. Journal of Physical Chemistry Letters, 2020, 11, 1675-1681.	2.1	25
39	Immunomodulatory Potential of Differently-Terminated Ultra-Small Silicon Carbide Nanoparticles. Nanomaterials, 2020, 10, 573.	1.9	7
40	Color centers in diamond for quantum applications. Semiconductors and Semimetals, 2020, , 1-36.	0.4	7
41	Thermal evolution of silicon carbide electronic bands. Physical Review Materials, 2020, 4, .	0.9	6
42	Size-Dependent Photocatalytic Activity of Cubic Boron Phosphide Nanocrystals in the Quantum Confinement Regime. Journal of Physical Chemistry C, 2019, 123, 23226-23235.	1.5	10
43	Optical Properties of Vanadium in 4 H Silicon Carbide for Quantum Technology. Physical Review Applied, 2019, 12, .	1.5	51
44	Optically Active Defects at the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mrow><mml:mi>Si</mml:mi><mml:mi mathvariant="normal">C</mml:mi></mml:mrow><mml:mo>/</mml:mo><mml:msub><mml:mrow><mml:mi>Si</mml:mi><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math> Interface. Physical Review Applied, 2019, 12, .	1.5	20
45	Electrical Charge State Manipulation of Single Silicon Vacancies in a Silicon Carbide Quantum Optoelectronic Device. Nano Letters, 2019, 19, 7173-7180.	4.5	61
46	Oxygenated (113) diamond surface for nitrogen-vacancy quantum sensors with preferential alignment and long coherence time from first principles. Carbon, 2019, 145, 273-280.	5.4	24
47	High-fidelity spin and optical control of single silicon-vacancy centres in silicon carbide. Nature Communications, 2019, 10, 1954.	5.8	167
48	Identification of divacancy and silicon vacancy qubits in 6H-SiC. Applied Physics Letters, 2019, 114, 112107.	1.5	28
49	Spectrally Stable Defect Qubits with no Inversion Symmetry for Robust Spin-To-Photon Interface. Physical Review Applied, 2019, 11, .	1.5	43
50	The (eg âŠ— eu) âŠ— Eg product Jahnâ€“Teller effect in the neutral group-IV vacancy quantum bits in diamond. Npj Computational Materials, 2019, 5, .	3.5	35
51	Ab initio theory of the nitrogen-vacancy center in diamond. Nanophotonics, 2019, 8, 1907-1943.	2.9	140
52	First-Principles Study on Photoluminescence Quenching of Divacancy in 4H SiC. Materials Science Forum, 2019, 963, 714-717.	0.3	1
53	Stabilization of point-defect spin qubits by quantum wells. Nature Communications, 2019, 10, 5607.	5.8	42
54	Electrically driven optical interferometry with spins in silicon carbide. Science Advances, 2019, 5, eaay0527.	4.7	55

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55	Evidence for Primal sp² Defects at the Diamond Surface: Candidates for Electron Trapping and Noise Sources. Advanced Materials Interfaces, 2019, 6, 1801449.	1.9	75
56	Color Centers in Hexagonal Boron Nitride Monolayers: A Group Theory and Ab Initio Analysis. ACS Photonics, 2018, 5, 1967-1976.	3.2	157
57	First principles predictions of magneto-optical data for semiconductor point defect identification: the case of divacancy defects in 4Hâ€“SiC. New Journal of Physics, 2018, 20, 023035.	1.2	39
58	Identification of the binding site between bovine serum albumin and ultrasmall SiC fluorescent biomarkers. Physical Chemistry Chemical Physics, 2018, 20, 13419-13429.	1.3	16
59	Room temperature solid-state quantum emitters in the telecom range. Science Advances, 2018, 4, eaar3580.	4.7	91
60	First-Principles Study of Charge Diffusion between Proximate Solid-State Qubits and Its Implications on Sensor Applications. Physical Review Letters, 2018, 120, 136401.	2.9	16
61	Strongly inhomogeneous distribution of spectral properties of silicon-vacancy color centers in nanodiamonds. New Journal of Physics, 2018, 20, 115002.	1.2	52
62	Ab Initio Spin-Strain Coupling Parameters of Divacancy Qubits in Silicon Carbide. Physical Review Applied, 2018, 10, .	1.5	23
63	Excitation properties of the divacancy in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>4</mml:mn><mml:mi>H</mml:mi></mml:mrow></mml:math> -SiC. Physical Review B, 2018, 98, .	1.1	14
64	Strongly anisotropic spin relaxation in the neutral silicon vacancy center in diamond. Physical Review B, 2018, 98, .	1.1	17
65	First principles calculation of spin-related quantities for point defect qubit research. Npj Computational Materials, 2018, 4, .	3.5	56
66	Photoluminescence, infrared, and Raman spectra of co-doped Si nanoparticles from first principles. Journal of Chemical Physics, 2018, 149, 154702.	1.2	6
67	Direct Observation of Transition from Solid-State to Molecular-Like Optical Properties in Ultrasmall Silicon Carbide Nanoparticles. Journal of Physical Chemistry C, 2018, 122, 26713-26721.	1.5	7
68	Theory of the optical spin-polarization loop of the nitrogen-vacancy center in diamond. Physical Review B, 2018, 98, .	1.1	59
69	Identification of nickel-vacancy defects by combining experimental and ab initio simulated photocurrent spectra. Physical Review B, 2018, 97, .	1.1	18
70	Spin-strain interaction in nitrogen-vacancy centers in diamond. Physical Review B, 2018, 98, .	1.1	77
71	Vibrational modes of negatively charged silicon-vacancy centers in diamond from ab initio calculations. Physical Review B, 2018, 98, .	1.1	27
72	Vibrational relaxation dynamics of the nitrogen-vacancy center in diamond. Physical Review B, 2018, 97, .	1.1	14

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73	Ab initio description of highly correlated states in defects for realizing quantum bits. Npj Quantum Materials, 2018, 3, .	1.8	60
74	AbÂInitio Magneto-Optical Spectrum of Group-IV Vacancy Color Centers in Diamond. Physical Review X, 2018, 8, .	2.8	104
75	Enhanced photoelectric detection of NV magnetic resonances in diamond under dual-beam excitation. Physical Review B, 2017, 95, .	1.1	34
76	Bright Roomâ€Temperature Singleâ€Photon Emission from Defects in Gallium Nitride. Advanced Materials, 2017, 29, 1605092.	11.1	102
77	Singleâ€Photon Emission: Bright Roomâ€Temperature Singleâ€Photon Emission from Defects in Gallium Nitride (Adv. Mater. 12/2017). Advanced Materials, 2017, 29, .	11.1	1
78	Nitrogen-Terminated Diamond (111) Surface for Room-Temperature Quantum Sensing and Simulation. Nano Letters, 2017, 17, 2294-2298.	4.5	65
79	Optical Gaps in Pristine and Heavily Doped Silicon Nanocrystals: DFT versus Quantum Monte Carlo Benchmarks. Journal of Chemical Theory and Computation, 2017, 13, 6061-6067.	2.3	11
80	Hybrid-DFTâ€‰â€‰+â€‰â€‰V_w method for band structure calculation of semiconducting transition metal compounds: the case of cerium dioxide. Journal of Physics Condensed Matter, 2017, 29, 454002.	0.7	5
81	Ab initio calculation of spin-orbit coupling for an NV center in diamond exhibiting dynamic Jahn-Teller effect. Physical Review B, 2017, 96, .	1.1	68
82	Protecting a Diamond Quantum Memory by Charge State Control. Nano Letters, 2017, 17, 5931-5937.	4.5	66
83	Characterization and formation of NV centers in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>3</mml:mn><mml:mi>C</mml:mi></mml:mrow><mm , and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>6</mml:mn><mml:mi>H</mml:mi></mml:mrow></mm SiC: An ab initio study. Physical Review B, 2017, 96, .	1.1	45
84	Harnessing no-photon exciton generation chemistry to engineer semiconductor nanostructures. Scientific Reports, 2017, 7, 10599.	1.6	13
85	Nitrogen-vacancy diamond sensor: novel diamond surfaces from ab initio simulations. MRS Communications, 2017, 7, 551-562.	0.8	25
86	All-optical hyperpolarization of electron and nuclear spins in diamond. Physical Review B, 2017, 96, .	1.1	11
87	Surface-Mediated Energy Transfer and Subsequent Photocatalytic Behavior in Silicon Carbide Colloid Solutions. Langmuir, 2017, 33, 14263-14268.	1.6	5
88	High-Throughput Study of Compositions and Optical Properties in Heavily Co-Doped Silicon Nanoparticles. Journal of Physical Chemistry C, 2017, 121, 27741-27750.	1.5	11
89	Ab initio theory of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">V</mml:mi></mml:mrow></mml:math> defect in diamond for quantum memory implementation. Physical Review B, 2017, 96, .	1.1	9
90	Identification of Si-vacancy related room-temperature qubits in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>4</mml:mn><mml:mi>H</mml:mi></mml:mrow></mml: silicon carbide. Physical Review B, 2017, 96, .	1.1	74

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91	Pulsed Photoelectric Coherent Manipulation and Detection of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">N</mml:mi><mml:mtext>â^'</mml:mtext><mml:mi>V</mml:mi></mml:mrow></mml:math> Center Spins in Diamond. Physical Review Applied, 2017, 7, .	1.5	27
92	Publisherâ€™s Note: Pulsed Photoelectric Coherent Manipulation and Detection of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">N</mml:mi><mml:mtext>â^'</mml:mtext><mml:mi>V</mml:mi></mml:mrow></mml:math> Center Spins In Diamond [Phys. Rev. Applied 7 , 044032 (2017)]. Physical Review Applied, 2017, 7, .	1.5	5
93	Isolated Spin Qubits in SiC with a High-Fidelity Infrared Spin-to-Photon Interface. Physical Review X, 2017, 7, .	2.8	125
94	Photoluminescence excitation spectroscopy of SiV^{â^'}and GeV^{â^'}color center in diamond. New Journal of Physics, 2017, 19, 063036.	1.2	75
95	The neutral silicon split-vacancy defect in diamond, a promising color center for quantum communication. , 2017, , .		0
96	Electronâ€"vibration coupling induced renormalization in the photoemission spectrum of diamondoids. Nature Communications, 2016, 7, 11327.	5.8	45
97	NV centers in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>3</mml:mn><mml:mi>C</mml:mi><mml:mo>,</mml:mo and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>6</mml:mn><mml:mi>H</mml:mi></mml:mrow></mml:m Optically detected magnetic resonances of nitrogen-vacancy ensembles in<mml:math 2016, 94, .	1.1	75
98	xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mmultiscripts><mml:mi mathvariant="normal">C</mml:mi><mml:mprescripts /><mml:none /><mml:mn>13</mml:mn></mml:mmultiscripts></mml:math>-enriched diamond. Physical Review B, 2016, 94, .	1.1	6
99	High-Fidelity Bidirectional Nuclear Qubit Initialization in SiC. Physical Review Letters, 2016, 117, 220503.	2.9	16
100	Characterization of oxygen defects in diamond by means of density functional theory calculations. Physical Review B, 2016, 94, .	1.1	23
101	Microscopic modeling of the effect of phonons on the optical properties of solid-state emitters. Physical Review B, 2016, 94, .	1.1	21
102	First Principles Identification of Divacancy Related Photoluminescence Lines in 4H and 6H-SiC. Materials Science Forum, 2016, 858, 322-325.	0.3	4
103	Determination of silicon and aluminum in silicon carbide nanocrystals by high-resolution continuum source graphite furnace atomic absorption spectrometry. Talanta, 2016, 147, 271-275.	2.9	17
104	Identification of Luminescence Centers in Molecular-Sized Silicon Carbide Nanocrystals. Journal of Physical Chemistry C, 2016, 120, 685-691.	1.5	31
105	Optical properties and Zeeman spectroscopy of niobium in silicon carbide. Physical Review B, 2015, 92, .	1.1	6
106	Complexes of silicon, vacancy, and hydrogen in diamond: A density functional study. Physical Review B, 2015, 92, .	1.1	30
107	Nitrogen Terminated Diamond. Advanced Materials Interfaces, 2015, 2, 1500079.	1.9	61
108	Dominant luminescence is not due to quantum confinement in molecular-sized silicon carbide nanocrystals. Nanoscale, 2015, 7, 10982-10988.	2.8	46

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109	Theoretical model of dynamic spin polarization of nuclei coupled to paramagnetic point defects in diamond and silicon carbide. Physical Review B, 2015, 92, .	1.1	59
110	Optical Polarization of Nuclear Spins in Silicon Carbide. Physical Review Letters, 2015, 114, 247603.	2.9	109
111	Spin and photophysics of carbon-antisite vacancy defect in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>4</mml:mn><mml:mi>H</mml:mi></mml:mrow></mml carbide: A potential quantum bit. Physical Review B, 2015, 91, .	1.1	50
112	Single-photon emitting diode in silicon carbide. Nature Communications, 2015, 6, 7783.	5.8	162
113	Coherent control of single spins in silicon carbide at room temperature. Nature Materials, 2015, 14, 164-168.	13.3	472
114	Two-site diamond-like point defects as new single-photon emitters. EPJ Web of Conferences, 2014, 78, 05001.	0.1	0
115	Publisher's Note: Formation of NV centers in diamond: A theoretical study based on calculated transitions and migration of nitrogen and vacancy related defects [Phys. Rev. B89, 075203 (2014)]. Physical Review B, 2014, 89, .	1.1	10
116	Electronic and optical properties of pure and modified diamondoids studied by many-body perturbation theory and time-dependent density functional theory. Journal of Chemical Physics, 2014, 141, 064308.	1.2	28
117	Characterization of the nitrogen split interstitial defect in wurtzite aluminum nitride using density functional theory. Journal of Applied Physics, 2014, 116, .	1.1	9
118	Exotic phase Si nanoparticles and Si-ZnS nanocomposites: New paradigms to improve the efficiency of MEG solar cells. , 2014, , .		0
119	Pressure and temperature dependence of the zero-field splitting in the ground state of NV centers in diamond: A first-principles study. Physical Review B, 2014, 90, .	1.1	97
120	First Principles Investigation of Divacancy in SiC Polytypes for Solid State Qubit Application. Materials Science Forum, 2014, 778-780, 499-502.	0.3	5
121	Theoretical and electron paramagnetic resonance studies of hyperfine interaction in nitrogen doped 4H and 6H SiC. Journal of Applied Physics, 2014, 115, .	1.1	17
122	Molecular-sized fluorescent nanodiamonds. Nature Nanotechnology, 2014, 9, 54-58.	15.6	229
123	A silicon carbide room-temperature single-photon source. Nature Materials, 2014, 13, 151-156.	13.3	439
124	Optoelectronic excitations and photovoltaic effect in strongly correlated materials. Physical Review B, 2014, 90, .	1.1	26
125	First principles study of point defects in SnS. Physical Chemistry Chemical Physics, 2014, 16, 26176-26183.	1.3	75
126	Germanium nanoparticles with non-diamond core structures for solar energy conversion. Journal of Materials Chemistry A, 2014, 2, 9820.	5.2	29

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127	Room Temperature Quantum Emission from Cubic Silicon Carbide Nanoparticles. ACS Nano, 2014, 8, 7938-7947.	7.3	89
128	Proper Surface Termination for Luminescent Near-Surface NV Centers in Diamond. Nano Letters, 2014, 14, 4772-4777.	4.5	125
129	Theoretical unification of hybrid-DFT and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mtext>DFT</mml:mtext><mml:mo>â€‰</mml:mo><mml:mo>+</mml:mo><mml:mo>U</mml:mo></mml:m for the treatment of localized orbitals. Physical Review B, 2014, 90, .	1.1	46
130	Formation of NV centers in diamond: A theoretical study based on calculated transitions and migration of nitrogen and vacancy related defects. Physical Review B, 2014, 89, .	1.1	149
131	Fluorine Modification of the Surface of Diamondoids: A Time-Dependent Density Functional Study. Journal of Physical Chemistry C, 2014, 118, 4410-4415.	1.5	12
132	Single nickel-related defects in molecular-sized nanodiamonds for multicolor bioimaging: an ab initio study. Nanoscale, 2014, 6, 12018-12025.	2.8	18
133	Solar Nanocomposites with Complementary Charge Extraction Pathways for Electrons and Holes: Si Embedded in ZnS. Physical Review Letters, 2014, 112, 106801.	2.9	22
134	Quantum-confined single photon emission at room temperature from SiC tetrapods. Nanoscale, 2014, 6, 10027-10032.	2.8	18
135	Computational design ofin vivobiomarkers. Journal of Physics Condensed Matter, 2014, 26, 143202.	0.7	13
136	The spinâ€“spin zero-field splitting tensor in the projector-augmented-wave method. Journal of Physics Condensed Matter, 2014, 26, 015305.	0.7	25
137	Chemical Transformation of Carboxyl Groups on the Surface of Silicon Carbide Quantum Dots. Journal of Physical Chemistry C, 2014, 118, 19995-20001.	1.5	16
138	Ab Initio Optoelectronic Properties of Silicon Nanoparticles: Excitation Energies, Sum Rules, and Tammâ€“Dancoff Approximation. Journal of Chemical Theory and Computation, 2014, 10, 3290-3298.	2.3	22
139	Electronic Structure of the Silicon Vacancy Color Center in Diamond. Physical Review Letters, 2014, 112, 036405.	2.9	312
140	Electrically and Mechanically Tunable Electron Spins in Silicon Carbide Color Centers. Physical Review Letters, 2014, 112, 187601.	2.9	152
141	Ab initiocharacterization of a Ni-related defect in diamond: The W8 center. Physical Review B, 2013, 87, .	1.1	15
142	Ab initiostudy of the split silicon-vacancy defect in diamond: Electronic structure and related properties. Physical Review B, 2013, 88, .	1.1	143
143	Limitations of the hybrid functional approach to electronic structure of transition metal oxides. Physical Review B, 2013, 88, .	1.1	24
144	Hyperfine coupling of point defects in semiconductors by hybrid density functional calculations: The role of core spin polarization. Physical Review B, 2013, 88, .	1.1	79

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145	Negative-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>U</mml:mi></mml:math>carbon vacancy in 4<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>H</mml:mi></mml:math>-SiC: Assessment of charge correction schemes and identification of the negative carbon vacancy at the quasicubic site. Physical Review B, 2013, 88, .	1.1	45
146	Comparative study of Si and Ge nanoparticles with exotic core phases for solar energy conversion. , 2013, , .		0
147	High-Pressure Core Structures of Si Nanoparticles for Solar Energy Conversion. Physical Review Letters, 2013, 110, 046804.	2.9	65
148	Increasing impact ionization rates in Si nanoparticles through surface engineering: A density functional study. Physical Review B, 2013, 87, .	1.1	24
149	Optically Controlled Switching of the Charge State of a Single Nitrogen-Vacancy Center in Diamond at Cryogenic Temperatures. Physical Review Letters, 2013, 110, 167402.	2.9	179
150	Role of screening in the density functional applied to transition-metal defects in semiconductors. Physical Review B, 2013, 87, .	1.1	35
151	Readout and control of a single nuclear spin with a metastable electron spin ancilla. Nature Nanotechnology, 2013, 8, 487-492.	15.6	64
152	Silicon carbide quantum dots for bioimaging. Journal of Materials Research, 2013, 28, 205-209.	1.2	40
153	Introducing Color Centers to Silicon Carbide Nanocrystals for In Vivo Biomarker Applications: A First Principles Study. Materials Science Forum, 2013, 740-742, 641-644.	0.3	1
154	Preparation of small silicon carbide quantum dots by wet chemical etching. Journal of Materials Research, 2013, 28, 44-49.	1.2	41
155	Electronic Configuration of Tungsten in 4H-, 6H-, and 15R-SiC. Materials Science Forum, 2012, 717-720, 211-216.	0.3	0
156	Local Thermal Expansion and the C-C Stretch Vibration of the Dicarbon Antisite in 4H SiC. Materials Science Forum, 2012, 717-720, 263-266.	0.3	1
157	Electron paramagnetic resonance and theoretical studies of Nb in 4H- and 6H-SiC. Journal of Applied Physics, 2012, 112, .	1.1	11
158	Enhancement of electron-nuclear hyperfine interaction at lattice defects in semiconducting single-walled carbon nanotubes studied byab initiodensity functional theory calculations. Physical Review B, 2012, 86, .	1.1	0
159	Preparation of Small Silicon Carbide Quantum Dots by Wet Chemical Etching. Materials Research Society Symposia Proceedings, 2012, 1468, 25.	0.1	0
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