Adam Gali

List of Publications by Citations

309 papers	9,799 citations	51 h-index	85 g-index
329 ext. papers	11,348 ext. citations	5 avg, IF	6.55 L-index

#	Paper	IF	Citations
309	A silicon carbide room-temperature single-photon source. *Nature Materials*, **2014**, 13, 151-6	27	349
308	Coherent control of single spins in silicon carbide at room temperature. *Nature Materials*, **2015**, 14, 164-8	27	347
307	Properties of nitrogen-vacancy centers in diamond: the group theoretic approach. *New Journal of Physics*, **2011**, 13, 025025	2.9	249
306	Electrically driven single-photon source at room temperature in diamond. *Nature Photonics*, **2012**, 6, 299-303	33.9	248
305	Electronic structure of the silicon vacancy color center in diamond. *Physical Review Letters*, **2014**, 112, 036405	7.4	225
304	Accurate defect levels obtained from the HSE06 range-separated hybrid functional. *Physical Review B*, **2010**, 81,	3.3	224
303	Ab initio supercell calculations on nitrogen-vacancy center in diamond: Electronic structure and hyperfine tensors. *Physical Review B*, **2008**, 77,	3.3	192
302	Molecular-sized fluorescent nanodiamonds. *Nature Nanotechnology*, **2014**, 9, 54-8	28.7	185
301	Direct correlation of crystal structure and optical properties in wurtzite/zinc-blende GaAs nanowire heterostructures. *Physical Review B*, **2011**, 83,	3.3	181
300	Theory of spin-conserving excitation of the N-V(-) center in diamond. *Physical Review Letters*, **2009**, 103, 186404	7.4	158
299	Divacancy in 4H-SiC. *Physical Review Letters*, **2006**, 96, 055501	7.4	151
298	Optically controlled switching of the charge state of a single nitrogen-vacancy center in diamond at cryogenic temperatures. *Physical Review Letters*, **2013**, 110, 167402	7.4	141
297	Defects in SiO2 as the possible origin of near interface traps in the SiC/SiO2 system: A systematic theoretical study. *Physical Review B*, **2005**, 72,	3.3	134
296	Dark states of single nitrogen-vacancy centers in diamond unraveled by single shot NMR. *Physical Review Letters*, **2011**, 106, 157601	7.4	130
295	Single-photon emitting diode in silicon carbide. *Nature Communications*, **2015**, 6, 7783	17.4	129
294	Ab initio study of nitrogen and boron substitutional impurities in single-wall SiC nanotubes. *Physical Review B*, **2006**, 73,	3.3	127
293	Electrically and mechanically tunable electron spins in silicon carbide color centers. *Physical Review Letters*, **2014**, 112, 187601	7.4	123

292	Theoretical study of the mechanism of dry oxidation of 4H-SiC. *Physical Review B*, **2005**, 71,	3.3	122
291	The mechanism of defect creation and passivation at the SiC/SiO2interface. *Journal Physics D: Applied Physics*, **2007**, 40, 6242-6253	3	120
290	Ab initio study of the split silicon-vacancy defect in diamond: Electronic structure and related properties. *Physical Review B*, **2013**, 88,	3.3	116
289	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,	3.3	113
288	Color Centers in Hexagonal Boron Nitride Monolayers: A Group Theory and Ab Initio Analysis. *ACS Photonics*, **2018**, 5, 1967-1976	6.3	100
287	High-fidelity spin and optical control of single silicon-vacancy centres in silicon carbide. *Nature Communications*, **2019**, 10, 1954	17.4	99
286	Ab initio density-functional supercell calculations of hydrogen defects in cubic SiC. *Physical Review B*, **2001**, 63,	3.3	99
285	Aggregation of carbon interstitials in silicon carbide: A theoretical study. *Physical Review B*, **2003**, 68,	3.3	94
284	Proper surface termination for luminescent near-surface NV centers in diamond. *Nano Letters*, **2014** , 14, 4772-7	11.5	92
283	13C hyperfine interactions in the nitrogen-vacancy centre in diamond. *New Journal of Physics*, **2011**, 13, 025021	2.9	90
282	Optical Polarization of Nuclear Spins in Silicon Carbide. *Physical Review Letters*, **2015**, 114, 247603	7.4	86
281	Excited states of the negatively charged nitrogen-vacancy color center in diamond. *Physical Review B*, **2010**, 81,	3.3	79
280	Isolated Spin Qubits in SiC with a High-Fidelity Infrared Spin-to-Photon Interface. *Physical Review X*, **2017**, 7,	9.1	78
279	Room temperature quantum emission from cubic silicon carbide nanoparticles. *ACS Nano*, **2014**, 8, 7938-47	13.7	77
278	Large-Scale Electronic Structure Calculations of Vacancies in 4H-SiC Using the Heyd-Scuseria-Ernzerhof Screened Hybrid Density Functional. *Materials Science Forum*, **2011**, 679-680, 261-264	0.4	75
277	Theoretical study of vacancy diffusion and vacancy-assisted clustering of antisites in SiC. *Physical Review B*, **2003**, 68,	3.3	72
276	Time-dependent density functional study on the excitation spectrum of point defects in semiconductors. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 1337-1346	1.3	70
275	The silicon vacancy in SiC. *Physica B: Condensed Matter*, **2009**, 404, 4354-4358	2.8	70

274	Theory of the neutral nitrogen-vacancy center in diamond and its application to the realization of a qubit. *Physical Review B*, **2009**, 79,	3.3	67
273	Bright Room-Temperature Single-Photon Emission from Defects in Gallium Nitride. *Advanced Materials*, **2017**, 29, 1605092	24	66
272	Identification of the carbon antisite-vacancy pair in 4H-SiC. *Physical Review Letters*, **2006**, 96, 145501	7.4	66
271	Correlation between the antisite pair and the DI center in SiC. *Physical Review B*, **2003**, 67,	3.3	66
270	Ab initio theory of the nitrogen-vacancy center in diamond. *Nanophotonics*, **2019**, 8, 1907-1943	6.3	65
269	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,	3.3	64
268	Room temperature solid-state quantum emitters in the telecom range. *Science Advances*, **2018**, 4, eaar3580	14.3	63
267	Ab Initio Magneto-Optical Spectrum of Group-IV Vacancy Color Centers in Diamond. *Physical Review X*, **2018**, 8,	9.1	61
266	Hyperfine coupling of point defects in semiconductors by hybrid density functional calculations: The role of core spin polarization. *Physical Review B*, **2013**, 88,	3.3	61
265	First principles study of point defects in SnS. *Physical Chemistry Chemical Physics*, **2014**, 16, 26176-83	3.6	60
264	NV centers in 3C,4H, and 6H silicon carbide: A variable platform for solid-state qubits and nanosensors. *Physical Review B*, **2016**, 94,	3.3	59
263	Intershell interaction in double walled carbon nanotubes: Charge transfer and orbital mixing. *Physical Review B*, **2008**, 77,	3.3	58
262	High-pressure core structures of Si nanoparticles for solar energy conversion. *Physical Review Letters*, **2013**, 110, 046804	7.4	56
261	Ab initio theory of the negatively charged boron vacancy qubit in hexagonal boron nitride. *Npj Computational Materials*, **2020**, 6,	10.9	55
260	EPR and theoretical studies of negatively charged carbon vacancy in 4H-SiC. *Physical Review B*, **2005**, 71,	3.3	53
259	Protecting a Diamond Quantum Memory by Charge State Control. *Nano Letters*, **2017**, 17, 5931-5937	11.5	51
258	Identification of Si-vacancy related room-temperature qubits in 4H silicon carbide. *Physical Review B*, **2017**, 96,	3.3	51
257	Photoluminescence excitation spectroscopy of SiV and GeV color center in diamond. *New Journal of Physics*, **2017**, 19, 063036	2.9	51

256	Spin-strain interaction in nitrogen-vacancy centers in diamond. *Physical Review B*, **2018**, 98,	3.3	50
255	Readout and control of a single nuclear spin with a metastable electron spin ancilla. *Nature Nanotechnology*, **2013**, 8, 487-92	28.7	49
254	Optical absorption of diamond nanocrystals from ab initio density-functional calculations. *Physical Review B*, **2009**, 80,	3.3	49
253	Nitrogen-Terminated Diamond (111) Surface for Room-Temperature Quantum Sensing and Simulation. *Nano Letters*, **2017**, 17, 2294-2298	11.5	48
252	Nitrogen Terminated Diamond. *Advanced Materials Interfaces*, **2015**, 2, 1500079	4.6	47
251	Theoretical model of dynamic spin polarization of nuclei coupled to paramagnetic point defects in diamond and silicon carbide. *Physical Review B*, **2015**, 92,	3.3	47
250	Ab initio calculation of spin-orbit coupling for an NV center in diamond exhibiting dynamic Jahn-Teller effect. *Physical Review B*, **2017**, 96,	3.3	46
249	Identification of individual C13 isotopes of nitrogen-vacancy center in diamond by combining the polarization studies of nuclear spins and first-principles calculations. *Physical Review B*, **2009**, 80,	3.3	43
248	EPR and theoretical studies of positively charged carbon vacancy in 4H SiC. *Physical Review B*, **2004**, 70,	3.3	43
247	Quantum guidelines for solid-state spin defects. *Nature Reviews Materials*,	73.3	43
246	Spin and photophysics of carbon-antisite vacancy defect in 4H silicon carbide: A potential quantum bit. *Physical Review B*, **2015**, 91,	3.3	41
245	Ab initio theoretical study of hydrogen and its interaction with boron acceptors and nitrogen donors in single-wall silicon carbide nanotubes. *Physical Review B*, **2007**, 75,	3.3	40
244	Evidence for Primal sp2 Defects at the Diamond Surface: Candidates for Electron Trapping and Noise Sources. *Advanced Materials Interfaces*, **2019**, 6, 1801449	4.6	40
243	Negative-U carbon vacancy in 4H-SiC: Assessment of charge correction schemes and identification of the negative carbon vacancy at the quasicubic site. *Physical Review B*, **2013**, 88,	3.3	39
242	Accurate single-particle determination of the band gap in silicon nanowires. *Physical Review B*, **2007**, 76,	3.3	39
241	The spin state of the neutral silicon vacancy in 3C SiC. *Applied Physics Letters*, **1999**, 75, 2103-2105	3.4	39
240	Ab initio description of highly correlated states in defects for realizing quantum bits. *Npj Quantum Materials*, **2018**, 3,	5	38
239	Characterization and formation of NV centers in 3C, 4H, and 6H SiC: An ab initio study. *Physical Review B*, **2017**, 96,	3.3	38

238	Accurate gap levels and their role in the reliability of other calculated defect properties. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 790-798	1.3	38
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236	Isolated oxygen defects in 3C- and 4H-SiC: A theoretical study. *Physical Review B*, **2002**, 66,	3.3	38
235	Dominant luminescence is not due to quantum confinement in molecular-sized silicon carbide nanocrystals. *Nanoscale*, **2015**, 7, 10982-8	7.7	37
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233	Material platforms for defect qubits and single-photon emitters. *Applied Physics Reviews*, **2020**, 7, 031308	17.3	37
232	Electrical Charge State Manipulation of Single Silicon Vacancies in a Silicon Carbide Quantum Optoelectronic Device. *Nano Letters*, **2019**, 19, 7173-7180	11.5	36
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230	Tuning the optical gap of nanometer-size diamond cages by sulfurization: a time-dependent density functional study. *Physical Review Letters*, **2012**, 108, 267401	7.4	36
229	Near-infrared luminescent cubic silicon carbide nanocrystals for in vivo biomarker applications: an ab initio study. *Nanoscale*, **2012**, 4, 7720-6	7.7	36
228	The absorption of oxygenated silicon carbide nanoparticles. *Journal of Chemical Physics*, **2010**, 133, 064705	3.9	35
227	Scanning transmission electron microscope observations of defects in as-grown and pre-strained Mo alloy fibers. *Acta Materialia*, **2011**, 59, 2172-2179	8.4	35
226	The absorption spectrum of hydrogenated silicon carbide nanocrystals from ab initio calculations. *Applied Physics Letters*, **2010**, 96, 051909	3.4	35
225	Identification of intrinsic defects in SiC: Towards an understanding of defect aggregates by combining theoretical and experimental approaches. *Physica Status Solidi (B): Basic Research*, **2008**, 245, 1281-1297	1.3	35
224	Theory of the optical spin-polarization loop of the nitrogen-vacancy center in diamond. *Physical Review B*, **2018**, 98,	3.3	35
223	Preparation of small silicon carbide quantum dots by wet chemical etching. *Journal of Materials Research*, **2013**, 28, 44-49	2.5	34
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221	Silicon carbide quantum dots for bioimaging. *Journal of Materials Research*, **2013**, 28, 205-209	2.5	33

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219	Identification of positively charged carbon antisite-vacancy pairs in 4H-SiC. *Physical Review B*, **2007**, 75,	3.3	33
218	Excitation properties of the divacancy in 4H-SiC. *Physical Review B*, **2018**, 98,	3.3	33
217	Optical Properties of Vanadium in 4H Silicon Carbide for Quantum Technology. *Physical Review Applied*, **2019**, 12,	4.3	32
216	Electrical characterization of metastable carbon clusters in SiC: A theoretical study. *Physical Review B*, **2006**, 73,	3.3	32
215	Electronic structure of boron-interstitial clusters in silicon. *Journal of Physics Condensed Matter*, **2005**, 17, S2141-S2153	1.8	32
214	Spectroscopic investigations of negatively charged tin-vacancy centres in diamond. *New Journal of Physics*, **2020**, 22, 013048	2.9	32
213	Characterization of luminescent silicon carbide nanocrystals prepared by reactive bonding and subsequent wet chemical etching. *Applied Physics Letters*, **2011**, 99, 213108	3.4	31
212	Electron-vibration coupling induced renormalization in the photoemission spectrum of diamondoids. *Nature Communications*, **2016**, 7, 11327	17.4	31
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210	First principles calculation of spin-related quantities for point defect qubit research. *Npj Computational Materials*, **2018**, 4,	10.9	31
209	Effect of oxygen on single-wall silicon carbide nanotubes studied by first-principles calculations. *Physical Review B*, **2009**, 80,	3.3	30
208	Vibronic States and Their Effect on the Temperature and Strain Dependence of Silicon-Vacancy Qubits in 4H-SiC. *Physical Review Applied*, **2020**, 13,	4.3	29
207	Role of screening in the density functional applied to transition-metal defects in semiconductors. *Physical Review B*, **2013**, 87,	3.3	29
206	Electron paramagnetic resonance and theoretical studies of shallow phosphorous centers in 3C-, 4H-, and 6H-SiC. *Physical Review B*, **2006**, 73,	3.3	29
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204	Excitation spectrum of point defects in semiconductors studied by time-dependent density functional theory. *Journal of Materials Research*, **2012**, 27, 897-909	2.5	28
203	Stabilization of point-defect spin qubits by quantum wells. *Nature Communications*, **2019**, 10, 5607	17.4	28

202	Theory of Neutral Divacancy in SiC: A Defect for Spintronics. *Materials Science Forum*, **2010**, 645-648, 395-397	0.4	27
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198	Spectrally Stable Defect Qubits with no Inversion Symmetry for Robust Spin-To-Photon Interface. *Physical Review Applied*, **2019**, 11,	4.3	26
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196	Defect states of substitutional oxygen in diamond. *Journal of Physics Condensed Matter*, **2001**, 13, 11607-11613	1.8	26
195	Enhanced photoelectric detection of NV magnetic resonances in diamond under dual-beam excitation. *Physical Review B*, **2017**, 95,	3.3	25
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189	Thermal stability of Cr□r3Si eutectic microstructures. *Acta Materialia*, **2009**, 57, 3823-3829	8.4	23
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186	The (eg ? eu) ? Eg product Jahn□Teller effect in the neutral group-IV vacancy quantum bits in diamond. *Npj Computational Materials*, **2019**, 5,	10.9	23
185	Complexes of silicon, vacancy, and hydrogen in diamond: A density functional study. *Physical Review B*, **2015**, 92,	3.3	22

184	Asymmetric split-vacancy defects in SiC polytypes: a combined theoretical and electron spin resonance study. *Physical Review Letters*, **2011**, 107, 195501	7.4	22
183	Ab initio supercell calculations on aluminum-related defects in SiC. *Physical Review B*, **2007**, 75,	3.3	22
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181	Optoelectronic excitations and photovoltaic effect in strongly correlated materials. *Physical Review B*, **2014**, 90,	3.3	20
180	The spin-spin zero-field splitting tensor in the projector-augmented-wave method. *Journal of Physics Condensed Matter*, **2014**, 26, 015305	1.8	20
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177	Solar nanocomposites with complementary charge extraction pathways for electrons and holes: Si embedded in ZnS. *Physical Review Letters*, **2014**, 112, 106801	7.4	19
176	Ab Initio Optoelectronic Properties of Silicon Nanoparticles: Excitation Energies, Sum Rules, and Tamm-Dancoff Approximation. *Journal of Chemical Theory and Computation*, **2014**, 10, 3290-8	6.4	19
175	Anharmonicity of the CH stretch mode in SiC: Unambiguous identification of hydrogen–silicon vacancy defect. *Applied Physics Letters*, **2002**, 80, 237-239	3.4	19
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172	Quantum-confined single photon emission at room temperature from SiC tetrapods. *Nanoscale*, **2014**, 6, 10027-32	7.7	17
171	Nitrogen-vacancy diamond sensor: novel diamond surfaces from ab initio simulations. *MRS Communications*, **2017**, 7, 551-562	2.7	17
170	Challenges for ab initio defect modeling. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **2008**, 154-155, 187-192	3.1	17
169	Diffusion of hydrogen in perfect, p-type doped, and radiation-damaged 4H-SiC. *Physical Review B*, **2004**, 69,	3.3	17
168	Optically Detected Magnetic Resonance in Neutral Silicon Vacancy Centers in Diamond via Bound Exciton States. *Physical Review Letters*, **2020**, 125, 237402	7.4	17
167	Theoretical and electron paramagnetic resonance studies of hyperfine interaction in nitrogen doped 4H and 6H SiC. *Journal of Applied Physics*, **2014**, 115, 073705	2.5	16

166	Theoretical study of small silicon clusters in 4H-SiC. *Physical Review B*, **2007**, 76,	3.3	16
165	Studies of boron–interstitial clusters in Si. *Journal of Physics Condensed Matter*, **2003**, 15, 4967-4977	1.8	16
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162	Identification of divacancy and silicon vacancy qubits in 6H-SiC. *Applied Physics Letters*, **2019**, 114, 112107	3.4	15
161	Single nickel-related defects in molecular-sized nanodiamonds for multicolor bioimaging: an ab initio study. *Nanoscale*, **2014**, 6, 12018-25	7.7	15
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159	Limits of the scaled shift correction to levels of interstitial defects in semiconductors. *Physical Review B*, **2007**, 75,	3.3	15
158	Hydrogen passivation of nitrogen in SiC. *Applied Physics Letters*, **2003**, 83, 1385-1387	3.4	15
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153	Chemical Transformation of Carboxyl Groups on the Surface of Silicon Carbide Quantum Dots. *Journal of Physical Chemistry C*, **2014**, 118, 19995-20001	3.8	14
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142	Fluorine Modification of the Surface of Diamondoids: A Time-Dependent Density Functional Study. *Journal of Physical Chemistry C*, **2014**, 118, 4410-4415	3.8	12
141	Optical identification and electronic configuration of tungsten in 4H- and 6H-SiC. *Physica B: Condensed Matter*, **2012**, 407, 1462-1466	2.8	12
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139	Some like it shallower: p-type doping in SiC. *Physica Status Solidi (B): Basic Research*, **2003**, 235, 139-145	1.3	12
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134	Harnessing no-photon exciton generation chemistry to engineer semiconductor nanostructures. *Scientific Reports*, **2017**, 7, 10599	4.9	11
133	Dicarbon antisite defect in n-type 4H-SiC. *Physical Review B*, **2009**, 79,	3.3	11
132	Modelling of stress-induced diamond nucleation. *Diamond and Related Materials*, **1995**, 4, 706-709	3.5	11
131	Stone-Wales defects in hexagonal boron nitride as ultraviolet emitters. *Npj Computational Materials*, **2020**, 6,	10.9	11

130	Room temperature coherent manipulation of single-spin qubits in silicon carbide with a high readout contrast. *National Science Review*,	10.8	11
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125	EPR and ab initio calculation study on the EI4 center in 4H- and 6H-SiC. *Physical Review B*, **2010**, 82,	3.3	10
124	Electron paramagnetic resonance and theoretical studies of Nb in 4H- and 6H-SiC. *Journal of Applied Physics*, **2012**, 112, 083711	2.5	10
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