

# Jrgen Furthmller

## List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

75 papers	45,694 citations	32 h-index	78 g-index
78 ext. papers	52,686 ext. citations	3.6 avg, IF	7.73 L-index

#	Paper	IF	Citations
75	Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set. <i>Computational Materials Science</i> , <b>1996</b> , 6, 15-50	3.2	41739
74	Ab initio Force Constant Approach to Phonon Dispersion Relations of Diamond and Graphite. <i>Europhysics Letters</i> , <b>1995</b> , 32, 729-734	1.6	568
73	Ultrasoft pseudopotentials applied to magnetic Fe, Co, and Ni: From atoms to solids. <i>Physical Review B</i> , <b>1997</b> , 56, 15629-15646	3.3	302
72	Vacancies in SiC: Influence of Jahn-Teller distortions, spin effects, and crystal structure. <i>Physical Review B</i> , <b>1999</b> , 59, 15166-15180	3.3	211
71	First-principles calculations of the thermodynamic and structural properties of strained In <sub>x</sub> Ga <sub>1-x</sub> N and Al <sub>x</sub> Ga <sub>1-x</sub> N alloys. <i>Physical Review B</i> , <b>2000</b> , 62, 2475-2485	3.3	172
70	Novel Reconstruction Mechanism for Dangling-Bond Minimization: Combined Method Surface Structure Determination of SiC(111)- (3 $\times$ 3). <i>Physical Review Letters</i> , <b>1998</b> , 80, 758-761	7.4	162
69	Electronic bands of III-V semiconductor polytypes and their alignment. <i>Physical Review B</i> , <b>2012</b> , 86,	3.3	126
68	Direct-bandgap emission from hexagonal Ge and SiGe alloys. <i>Nature</i> , <b>2020</b> , 580, 205-209	50.4	124
67	Accurate band gaps of AlGaN, InGaN, and AlInN alloys calculations based on LDA-1/2 approach. <i>Applied Physics Letters</i> , <b>2011</b> , 98, 151907	3.4	118
66	Do we know the fundamental energy gap of InN?. <i>Journal of Crystal Growth</i> , <b>2002</b> , 246, 315-319	1.6	112
65	Structural and electronic properties of rhodium surfaces: an ab initio approach. <i>Surface Science</i> , <b>1996</b> , 346, 300-321	1.8	110
64	Extreme softening of Vanderbilt pseudopotentials: General rules and case studies of first-row and d-electron elements. <i>Physical Review B</i> , <b>2000</b> , 61, 4576-4587	3.3	98
63	Dynamics and polarization of group-III nitride lattices: A first-principles study. <i>Physical Review B</i> , <b>2000</b> , 62, 8003-8011	3.3	98
62	High-precision determination of atomic positions in crystals: The case of 6H- and 4H-SiC. <i>Physical Review B</i> , <b>1998</b> , 57, 2647-2650	3.3	93
61	Phase separation suppression in InGaN epitaxial layers due to biaxial strain. <i>Applied Physics Letters</i> , <b>2002</b> , 80, 769-771	3.4	92
60	Energy gap and optical properties of In <sub>x</sub> Ga <sub>1-x</sub> N. <i>Physica Status Solidi A</i> , <b>2003</b> , 195, 628-633		86
59	Stacking faults in group-IV crystals: An ab initio study. <i>Physical Review B</i> , <b>1998</b> , 58, 1326-1330	3.3	78

58	Si-rich SiC(111)/(0001)3B and 3B surfaces: A Mott-Hubbard picture. <i>Physical Review B</i> , <b>1998</b> , 58, 13712-13716	3.3	71
57	Dielectric tensor of monoclinic Ga <sub>2</sub> O <sub>3</sub> single crystals in the spectral range 0.58-5 eV. <i>APL Materials</i> , <b>2015</b> , 3, 106106	5.7	65
56	Lattice parameter and energy band gap of cubic Al <sub>x</sub> Ga <sub>1-x</sub> In <sub>1-x</sub> N quaternary alloys. <i>Applied Physics Letters</i> , <b>2003</b> , 83, 890-892	3.4	65
55	Bond-rotation versus bond-contraction relaxation of (110) surfaces of group-III nitrides. <i>Physical Review B</i> , <b>1998</b> , 58, R1722-R1725	3.3	64
54	Structural and Electronic Properties of Clean and Hydrogenated Diamond (100) Surfaces. <i>Europhysics Letters</i> , <b>1994</b> , 28, 659-664	1.6	61
53	Spin-orbit effects in structural and electronic properties for the solid state of the group-14 elements from carbon to superheavy element 114. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	57
52	Spin state of vacancies: From magnetic Jahn-Teller distortions to multiplets. <i>Physical Review B</i> , <b>2000</b> , 62, 6854-6857	3.3	57
51	Band-structure and optical-transition parameters of wurtzite MgO, ZnO, and CdO from quasiparticle calculations. <i>Physica Status Solidi (B): Basic Research</i> , <b>2009</b> , 246, 2150-2153	1.3	56
50	Strain influence on valence-band ordering and excitons in ZnO: An ab initio study. <i>Applied Physics Letters</i> , <b>2007</b> , 91, 241915	3.4	52
49	Electronic and optical properties of Mg <sub>x</sub> Zn <sub>1-x</sub> O and Cd <sub>x</sub> Zn <sub>1-x</sub> O from ab initio calculations. <i>New Journal of Physics</i> , <b>2011</b> , 13, 085012	2.9	49
48	Theory of magnetostriction in amorphous and polycrystalline ferromagnets. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1987</b> , 69, 79-88	2.8	42
47	Gap bowing and Stokes shift in In <sub>x</sub> Ga <sub>1-x</sub> N alloys: First-principles studies. <i>Applied Physics Letters</i> , <b>2002</b> , 80, 1394-1396	3.4	41
46	Theoretical investigation of edge dislocations in AlN. <i>Applied Physics Letters</i> , <b>1998</b> , 72, 3467-3469	3.4	39
45	Spinodal decomposition in B <sub>x</sub> Ga <sub>1-x</sub> N and B <sub>x</sub> Al <sub>1-x</sub> N alloys. <i>Applied Physics Letters</i> , <b>2002</b> , 80, 1177-1179	3.4	37
44	Structural features and electronic properties of group-III-, group-IV-, and group-V-doped Si nanocrystallites. <i>Journal of Physics Condensed Matter</i> , <b>2007</b> , 19, 466211	1.8	33
43	Phase diagram, chemical bonds, and gap bowing of cubic In <sub>x</sub> Al <sub>1-x</sub> N alloys: Ab initio calculations. <i>Journal of Applied Physics</i> , <b>2002</b> , 92, 7109-7113	2.5	31
42	On the nature of the D1-defect center in SiC: A photoluminescence study of layers grown by solid-source molecular-beam epitaxy. <i>Applied Physics Letters</i> , <b>2001</b> , 78, 2512-2514	3.4	31
41	Optical properties of Si and Ge nanocrystals: Parameter-free calculations. <i>Physica Status Solidi (B): Basic Research</i> , <b>2005</b> , 242, 3053-3063	1.3	30

40	Electron correlation effects on SiC(111) and SiC(0001) surfaces. <i>Journal of Physics Condensed Matter</i> , <b>2004</b> , 16, S1721-S1732	1.8	26
39	Theory of magnetostriction in amorphous and polycrystalline ferromagnets. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1987</b> , 69, 89-98	2.8	26
38	Magnetic properties of MnN: Influence of strain and crystal structure. <i>Applied Physics Letters</i> , <b>2005</b> , 86, 164105	3.4	25
37	Structural and electronic properties of $\text{HfN}$ nanocrystals from first principles. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	24
36	Influence of oxygen on optical properties of Si nanocrystallites. <i>Applied Physics Letters</i> , <b>2005</b> , 87, 143113	3.4	24
35	Polytypic transformations in SiC: An ab initio study. <i>Physical Review B</i> , <b>1999</b> , 60, 13261-13264	3.3	22
34	GaMnAs: Position of Mn-d levels and majority spin band gap predicted from GGA-1/2 calculations. <i>Applied Physics Letters</i> , <b>2012</b> , 100, 202408	3.4	21
33	Influence of Polymorphism on the Electronic Structure of $\text{Ga}_2\text{O}_3$ . <i>Chemistry of Materials</i> , <b>2020</b> , 32, 8460-8470	3.4	21
32	Quasiparticle and excitonic effects in the optical spectra of diamond, SiC, Si, GaP, GaAs, InP, and AlN. <i>Physica Status Solidi (B): Basic Research</i> , <b>2005</b> , 242, 2720-2728	1.3	20
31	Initial stages of III-nitride growth. <i>Applied Physics Letters</i> , <b>1999</b> , 74, 3851-3853	3.4	20
30	Accurate electronic and optical properties of hexagonal germanium for optoelectronic applications. <i>Physical Review Materials</i> , <b>2019</b> , 3,	3.2	19
29	Distribution of cations in wurtzitic $\text{In}_x\text{Ga}_{1-x}\text{N}$ and $\text{In}_x\text{Al}_{1-x}\text{N}$ alloys: Consequences for energetics and quasiparticle electronic structures. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	18
28	Native defects and complexes in SiC. <i>Journal of Physics Condensed Matter</i> , <b>2001</b> , 13, 9027-9037	1.8	17
27	Carbon vacancy in SiC: A negative- U system. <i>Europhysics Letters</i> , <b>1998</b> , 44, 309-314	1.6	17
26	Polytypism and surface structure of SiC. <i>Diamond and Related Materials</i> , <b>1997</b> , 6, 1346-1348	3.5	16
25	Intravacancy transition energies in $3\text{C-SiC}$ and $4\text{H-SiC}$ . <i>Physical Review B</i> , <b>2000</b> , 61, 13655-13658	3.3	14
24	Theory of atomic level magnetostrictive deformations and stresses in amorphous ferromagnets. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1988</b> , 75, 225-232	2.8	14
23	Intrinsic spin Hall conductivity in one-, two-, and three-dimensional trivial and topological systems. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	13

22	Electronic and optical properties of cadmium fluoride: The role of many-body effects. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	13
21	Ab initio calculation of optical properties with excitonic effects in wurtzite $\text{In}_x\text{Ga}_{1-x}\text{N}$ and $\text{In}_x\text{Al}_{1-x}\text{N}$ alloys. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	13
20	Influence of screening dynamics on excitons in $\text{Ga}_2\text{O}_3$ polymorphs. <i>Applied Physics Letters</i> , <b>2019</b> , 114, 122101	3.4	12
19	Phase Separation, Gap Bowing, and Structural Properties of Cubic $\text{In}_x\text{Al}_{1-x}\text{N}$ . <i>Physica Status Solidi (B): Basic Research</i> , <b>2002</b> , 234, 956-960	1.3	12
18	Band structure and electron gas of In chains on Si(111). <i>Surface Science</i> , <b>2005</b> , 589, 77-90	1.8	12
17	Local magnetic anisotropy and magnetostriction of amorphous ferromagnets. <i>Physica B: Condensed Matter</i> , <b>1990</b> , 161, 225-231	2.8	12
16	Various contributions to magnetostriction in amorphous and polycrystalline ferromagnets. <i>Journal of Magnetism and Magnetic Materials</i> , <b>1988</b> , 72, 6-12	2.8	11
15	Optical absorption and emission of $\text{In}$ nanocrystals from first principles. <i>Nanotechnology</i> , <b>2013</b> , 24, 405702	3.4	10
14	Surface Energies and Surface Dipoles at III-Nitride(111) Surfaces in Dependence on Stoichiometry. <i>Physica Status Solidi (B): Basic Research</i> , <b>1999</b> , 216, 675-678	1.3	10
13	Stoichiometry and surface reconstructions of (001) surfaces of silicon carbide. <i>Surface Science</i> , <b>1996</b> , 352-354, 55-59	1.8	10
12	Are amorphous ferromagnets with $B=0$ magnetostrictive on a local scale?. <i>Applied Physics Letters</i> , <b>1991</b> , 59, 2049-2051	3.4	9
11	Quantization of spin Hall conductivity in two-dimensional topological insulators versus symmetry and spin-orbit interaction. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	9
10	On the Change of Magnetostriction by Field Annealing of Amorphous Ferromagnetic Alloys. <i>Physica Status Solidi A</i> , <b>1990</b> , 117, K71-K75		6
9	Nonparabolicity and excitons in optical absorption of InN. <i>Journal of Crystal Growth</i> , <b>2006</b> , 288, 294-297	1.6	5
8	Efficient strain-induced light emission in lonsdaleite germanium. <i>Physical Review Materials</i> , <b>2021</b> , 5,	3.2	5
7	Screening and band structure effects on quasi-one-dimensional transport in periodically modulated graphene. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	4
6	Dielectric and lattice-dynamical properties of III-nitrides. <i>Journal of Electronic Materials</i> , <b>2000</b> , 29, 281-284	4	4
5	One- and two-particle effects in the electronic and optical spectra of barium fluoride. <i>Journal of Physics Condensed Matter</i> , <b>2014</b> , 26, 125501	1.8	3

4	Electronic and Optical Properties of Small Metal Fluoride Clusters. <i>ACS Omega</i> , <b>2020</b> , 5, 13268-13277	3.9	2
3	From pseudo-direct hexagonal germanium to direct silicon-germanium alloys. <i>Physical Review Materials</i> , <b>2021</b> , 5,	3.2	2
2	In4d and Ga3d levels in In <sub>x</sub> X <sub>1-x</sub> N (X = Ga, Al) alloys. <i>Applied Physics Letters</i> , <b>2013</b> , 102, 172105	3.4	1
1	Classical versus ab initio structural relaxation: electronic excitations and optical properties of Ge nanocrystals embedded in an SiC matrix. <i>Journal of Physics Condensed Matter</i> , <b>2005</b> , 17, 643-651	1.8	1