Friedhelm Bechstedt

List of Publications by Citations

594 papers	25,972 citations	82 h-index	135 g-index
606 ext. papers	27,986 ext. citations	3.2 avg, IF	7.12 L-index

#	Paper	IF	Citations
594	Linear optical properties in the projector-augmented wave methodology. *Physical Review B*, **2006**, 73,	3.3	1857
593	Absorption and Emission of Hexagonal InN. Evidence of Narrow Fundamental Band Gap. *Physica Status Solidi (B): Basic Research*, **2002**, 229, r1-r3	1.3	862
592	Semiempirical van der Waals correction to the density functional description of solids and molecular structures. *Physical Review B*, **2006**, 73,	3.3	641
591	Quasiparticle band structure based on a generalized Kohn-Sham scheme. *Physical Review B*, **2007**, 76,	3.3	441
590	Properties of strained wurtzite GaN and AlN: Ab initio studies. *Physical Review B*, **2002**, 66,	3.3	338
589	First-principles study of ground- and excited-state properties of MgO, ZnO, and CdO polymorphs. *Physical Review B*, **2006**, 73,	3.3	325
588	Band gap, electronic structure, and surface electron accumulation of cubic and rhombohedral In2O3. *Physical Review B*, **2009**, 79,	3.3	323
587	Absolute surface energies of group-IV semiconductors: Dependence on orientation and reconstruction. *Physical Review B*, **2002**, 65,	3.3	318
586	Attracted by long-range electron correlation: adenine on graphite. *Physical Review Letters*, **2005**, 95, 186101	7.4	259
585	Band Gap of InN and In-Rich InxGa1□N alloys (0.36 Physica Status Solidi (B): Basic Research, **2002**, 230, R4-R6	1.3	255
584	Band Gap of Hexagonal InN and InGaN Alloys. *Physica Status Solidi (B): Basic Research*, **2002**, 234, 787-795	1.3	238
583	Optical properties of semiconductors using projector-augmented waves. *Physical Review B*, **2001**, 63,	3.3	238
582	Direct band gap wurtzite gallium phosphide nanowires. *Nano Letters*, **2013**, 13, 1559-63	11.5	230
581	Quasiparticle band structures of the antiferromagnetic transition-metal oxides MnO, FeO, CoO, and NiO. *Physical Review B*, **2009**, 79,	3.3	217
580	Vacancies in SiC: Influence of Jahn-Teller distortions, spin effects, and crystal structure. *Physical Review B*, **1999**, 59, 15166-15180	3.3	211
579	Polytypism and Properties of Silicon Carbide. *Physica Status Solidi (B): Basic Research*, **1997**, 202, 35-62	1.3	201
578	Indium-oxide polymorphs from first principles: Quasiparticle electronic states. *Physical Review B*, **2008**, 77,	3.3	201

577	Ab initio lattice dynamics of BN and AlN: Covalent versus ionic forces. *Physical Review B*, **1997**, 56, 7404-7415	3.3	192
576	Origin of electron accumulation at wurtzite InN surfaces. *Physical Review B*, **2004**, 69,	3.3	189
575	Principles of Surface Physics. *Advanced Texts in Physics*, **2003**,		178
574	First-principles calculations of the thermodynamic and structural properties of strained InxGa1−xN and AlxGa1−xN alloys. *Physical Review B*, **2000**, 62, 2475-2485	3.3	172
573	Novel Reconstruction Mechanism for Dangling-Bond Minimization: Combined Method Surface Structure Determination of SiC(111)- (3×3). *Physical Review Letters*, **1998**, 80, 758-761	7.4	162
572	Phonon deformation potentials of α-GaN and -AlN: An ab initio calculation. *Applied Physics Letters*, **2000**, 77, 346-348	3.4	161
571	Ab initio study of structural, dielectric, and dynamical properties of GaN. *Physical Review B*, **1998**, 57, 7043-7049	3.3	156
570	First-principles calculations of gap bowing in InxGa1−xN and InxAl1−xN alloys: Relation to structural and thermodynamic properties. *Physical Review B*, **2002**, 65,	3.3	155
569	Branch-point energies and band discontinuities of III-nitrides and III-/II-oxides from quasiparticle band-structure calculations. *Applied Physics Letters*, **2009**, 94, 012104	3.4	150
568	Massive Dirac quasiparticles in the optical absorbance of graphene, silicene, germanene, and tinene. *Journal of Physics Condensed Matter*, **2013**, 25, 395305	1.8	134
567	Infrared absorbance of silicene and germanene. *Applied Physics Letters*, **2012**, 100, 261906	3.4	134
566	Optical properties of two-dimensional honeycomb crystals graphene, silicene, germanene, and tinene from first principles. *New Journal of Physics*, **2014**, 16, 105007	2.9	131
565	First-principles optical spectra for F centers in MgO. *Physical Review Letters*, **2012**, 108, 126404	7.4	131
564	Tin dioxide from first principles: Quasiparticle electronic states and optical properties. *Physical Review B*, **2011**, 83,	3.3	129
563	Nonlocality and many-body effects in the optical properties of semiconductors. *Physical Review B*, **1996**, 53, 9797-9808	3.3	128
562	Optical and energy-loss spectra of MgO, ZnO, and CdO from ab initio many-body calculations. *Physical Review B*, **2009**, 80,	3.3	127
561	Electronic bands of III-V semiconductor polytypes and their alignment. *Physical Review B*, **2012**, 86,	3.3	126
560	Model GW band structure of InAs and GaAs in the wurtzite phase. *Physical Review B*, **2007**, 75,	3.3	126

559	Direct-bandgap emission from hexagonal Ge and SiGe alloys. *Nature*, **2020**, 580, 205-209	50.4	124
558	Electronic properties of cubic and hexagonal SiC polytypes from ab initio calculations. *Physical Review B*, **1994**, 50, 10761-10768	3.3	123
557	An efficient method for calculating quasiparticle energies in semiconductors. *Solid State Communications*, **1992**, 84, 765-770	1.6	123
556	Analytical treatment of band-gap underestimates in the local-density approximation. *Physical Review B*, **1988**, 38, 7710-7716	3.3	123
555	Universal infrared absorbance of two-dimensional honeycomb group-IV crystals. *Physical Review B*, **2013**, 87,	3.3	122
554	Influence of atomic relaxations on the structural properties of SiC polytypes from ab initio calculations. *Physical Review B*, **1994**, 50, 17037-17046	3.3	122
553	Efficient O(N2) method to solve the Bethe-Salpeter equation. *Physical Review B*, **2003**, 67,	3.3	121
552	Coulombic amino group-metal bonding: adsorption of adenine on Cu110. *Physical Review Letters*, **2005**, 94, 236102	7.4	120
551	Charge transport in organic crystals: Theory and modelling. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 511-525	1.3	118
550	Quasiparticle bands and spectra of Ga2O3 polymorphs. *Physical Review B*, **2016**, 93,	3.3	117
549	Phonons in ternary group-III nitride alloys. *Physical Review B*, **2000**, 61, 6091-6105	3.3	115
548	Theory of charge transport in organic crystals: Beyond Holstein□ small-polaron model. *Physical Review B*, **2009**, 79,	3.3	114
547	Optical absorption of water: coulomb effects versus hydrogen bonding. *Physical Review Letters*, **2005**, 94, 037404	7.4	114
546	Numerical calculation of the optical absorption in semiconductor quantum structures. *Physical Review B*, **1996**, 54, 11592-11601	3.3	114
545	Properties of hexagonal polytypes of group-IV elements from first-principles calculations. *Physical Review B*, **2002**, 66,	3.3	113
544	Do we know the fundamental energy gap of InN?. *Journal of Crystal Growth*, **2002**, 246, 315-319	1.6	112
543	Model dielectric function for semiconductors. *Physical Review B*, **1993**, 47, 9892-9895	3.3	111
542	Unit cell structure of crystal polytypes in InAs and InSb nanowires. *Nano Letters*, **2011**, 11, 1483-9	11.5	110

541	Heterocrystalline structures: New types of superlattices?. *Physical Review Letters*, **1995**, 75, 2180-2183	7.4	110
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539	Ab-initio theory of semiconductor band structures: New developments and progress. *Physica Status Solidi (B): Basic Research*, **2009**, 246, 1877-1892	1.3	107
538	Shape of free and constrained group-IV crystallites: Influence of surface energies. *Physical Review B* , **2005**, 72,	3.3	107
537	Valence-band electronic structure of CdO, ZnO, and MgO from x-ray photoemission spectroscopy and quasi-particle-corrected density-functional theory calculations. *Physical Review B*, **2009**, 79,	3.3	106
536	Quasiparticle band structure of silicon carbide polytypes. *Physical Review B*, **1995**, 52, 10897-10905	3.3	105
535	Hund's Rule-Driven Dzyaloshinskii-Moriya Interaction at 3d-5d Interfaces. *Physical Review Letters*, **2016**, 117, 247202	7.4	105
534	Band structures and optical spectra of InN polymorphs: Influence of quasiparticle and excitonic effects. *Physical Review B*, **2005**, 72,	3.3	102
533	Pressure-dependent properties of SiC polytypes. *Physical Review B*, **1996**, 53, 13400-13413	3.3	102
532	Reflectance Anisotropy of GaAs(100): Theory and Experiment. *Physical Review Letters*, **1998**, 81, 721-724	7.4	101
531	Strong excitons in novel two-dimensional crystals: Silicane and germanane. *Europhysics Letters*, **2012**, 98, 37004	1.6	100
530	Stability and electronic structure of two-dimensional allotropes of group-IV materials. *Physical Review B*, **2015**, 92,	3.3	98
529	Extreme softening of Vanderbilt pseudopotentials: General rules and case studies of first-row and d-electron elements. *Physical Review B*, **2000**, 61, 4576-4587	3.3	98
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527	Free-carrier absorption in nitrides from first principles. *Physical Review B*, **2010**, 81,	3.3	97
526	Efficient O(N2) approach to solve the Bethe-Salpeter equation for excitonic bound states. *Physical Review B*, **2008**, 78,	3.3	97
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520	High-precision determination of atomic positions in crystals: The case of 6H- and 4H-SiC. *Physical Review B*, **1998**, 57, 2647-2650	3.3	93
519	Phase separation suppression in InGaN epitaxial layers due to biaxial strain. *Applied Physics Letters*, **2002**, 80, 769-771	3.4	92
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517	Optical properties of Ge and Si nanocrystallites from ab initio calculations. II. Hydrogenated nanocrystallites. *Physical Review B*, **2002**, 65,	3.3	88
516	Geometry and electronic structure of GaAs(001)(2 x 4) reconstructions. *Physical Review B*, **1996**, 54, 16742-16748	3.3	88
515	Energy gap and optical properties of InxGa1-xN. *Physica Status Solidi A*, **2003**, 195, 628-633		86
514	Raman spectra of isotopic GaN. *Physical Review B*, **1997**, 56, 14399-14406	3.3	84
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507	Ground- and excited-state properties of DNA base molecules from plane-wave calculations using ultrasoft pseudopotentials. *Journal of Computational Chemistry*, **2004**, 25, 112-22	3.5	79
506	Stacking faults in group-IV crystals: An ab initio study. *Physical Review B*, **1998**, 58, 1326-1330	3.3	78

505	Crystalline and magnetic anisotropy of the 3d-transition metal monoxides MnO, FeO, CoO, and NiO. *Physical Review B*, **2012**, 86,	3.3	77
504	Ab initio theory of excitons and optical properties for spin-polarized systems: Application to antiferromagnetic MnO. *Physical Review B*, **2008**, 77,	3.3	74
503	Surface phase diagram of (2×4) and (4×2) reconstructions of GaAs(001). *Physical Review B*, **2000**, 62, 8087-8091	3.3	74
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499	Si-rich SiC(111)/(0001)3×3 and 3×3 surfaces: A Mott-Hubbard picture. *Physical Review B*, **1998**, 58, 13712-13716	3.3	71
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496	Influence of polytypism on thermal properties of silicon carbide. *Physical Review B*, **1996**, 54, 1791-1798	3.3	68
495	Band structure of ZnO from resonant x-ray emission spectroscopy. *Physical Review B*, **2008**, 78,	3.3	67
494	Raman studies on phonon modes in cubic AlGaN alloy. *Applied Physics Letters*, **1999**, 74, 191-193	3.4	67
493	Origin of Dirac-cone-like features in silicon structures on Ag(111) and Ag(110). *Journal of Applied Physics*, **2013**, 114, 113710	2.5	65
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487	Structure- and spin-dependent excitation energies and lifetimes of Si and Ge nanocrystals from ab initio calculations. *Physical Review B*, **2004**, 69,	3.3	62
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472	Spin state of vacancies: From magnetic Jahn-Teller distortions to multiplets. *Physical Review B*, **2000**, 62, 6854-6857	3.3	57
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461	III-V(110) surface dynamics from an ab initio frozen-phonon approach. *Physical Review B*, **1995**, 52, 2001-2007	3.3	55
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454	Strain influence on valence-band ordering and excitons in ZnO: An ab initio study. *Applied Physics Letters*, **2007**, 91, 241915	3.4	52
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450	GaAs(001): Surface Structure and Optical Properties. *Physica Status Solidi A*, **2001**, 188, 1401-1409		51
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447	Validity of effective-medium theory for optical properties of embedded nanocrystallites from ab initio supercell calculations. *Physical Review B*, **2003**, 67,	3.3	50
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439	Atomic Structure of the Sb-Stabilized GaAs(100)-(2 x 4) Surface. *Physical Review Letters*, **1996**, 77, 4402-4405	7.4	47
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