Friedhelm Bechstedt

List of Publications by Year in Descending Order

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	Optical properties of Xenes **2022**, 319-352		
593	From pseudo-direct hexagonal germanium to direct silicon-germanium alloys. *Physical Review Materials*, **2021**, 5,	3.2	2
592	Optical Signatures of Dirac Electrodynamics for hBN-Passivated Silicene on Au(111). *Nano Letters*, **2021**, 21, 5301-5307	11.5	3
591	Efficient strain-induced light emission in lonsdaleite germanium. *Physical Review Materials*, **2021**, 5,	3.2	5
590	Beyond graphene: Clean, hydrogenated and halogenated silicene, germanene, stanene, and plumbene. *Progress in Surface Science*, **2021**, 96, 100615	6.6	5
589	Electronic and Optical Properties of Small Metal Fluoride Clusters. *ACS Omega*, **2020**, 5, 13268-13277	3.9	2
588	Giant excitonic absorption and emission in two-dimensional group-III nitrides. *Scientific Reports*, **2020**, 10, 10719	4.9	11
587	Direct-bandgap emission from hexagonal Ge and SiGe alloys. *Nature*, **2020**, 580, 205-209	50.4	124
586	Starke Lichtemission in hexagonalen Ge- und SiGe-Halbleitern. *Physik in Unserer Zeit*, **2020**, 51, 216-217	0.1	
585	Influence of anisotropy, tilt and pairing of Weyl nodes: the Weyl semimetals TaAs, TaP, NbAs and NbP. *European Physical Journal B*, **2020**, 93, 1	1.2	1
584	Charge qubit in van der Waals heterostructures. *Physical Review B*, **2019**, 100,	3.3	10
583	Out-of-plane excitons in two-dimensional crystals. *Physical Review B*, **2019**, 99,	3.3	17
582	Influence of screening dynamics on excitons in Ga2O3 polymorphs. *Applied Physics Letters*, **2019**, 114, 122101	3.4	12
581	Organic Molecule Adsorption on Stepped Si(Au Surfaces: Role of Functional Group on Geometry and Electronic Structure. *Physica Status Solidi (B): Basic Research*, **2019**, 256, 1800653	1.3	
580	Forbidden Band-Edge Excitons of Wurtzite-GaP: A Theoretical View. *Physica Status Solidi (B): Basic Research*, **2019**, 256, 1800238	1.3	10
579	Accurate electronic and optical properties of hexagonal germanium for optoelectronic applications. *Physical Review Materials*, **2019**, 3,	3.2	19
578	Lattice vibrations and electronic properties of GaSe nanosheets from first principles. *Physical Review Materials*, **2019**, 3,	3.2	1

577	Quantization of spin Hall conductivity in two-dimensional topological insulators versus symmetry and spin-orbit interaction. *Physical Review B*, **2019**, 100,	3.3	9
576	Honeycomb silicon on alumina: Massless Dirac fermions in silicene on substrate. *Physical Review B*, **2019**, 100,	3.3	7
575	Trends on band alignments: Validity of Anderson's rule in SnS2- and SnSe2-based van der Waals heterostructures. *Physical Review B*, **2018**, 97,	3.3	40
574	Selective adsorption of toluene-3,4-dithiol on Si(553)-Au surfaces. *Physical Review B*, **2018**, 97,	3.3	6
573	Efficient Green Emission from Wurtzite Al InP Nanowires. *Nano Letters*, **2018**, 18, 3543-3549	11.5	14
572	Validity of Weyl fermion picture for transition metals monopnictides TaAs, TaP, NbAs, and NbP from ab initio studies. *Scientific Reports*, **2018**, 8, 3534	4.9	23
571	Electronic excitations stabilized by a degenerate electron gas in semiconductors. *Communications Physics*, **2018**, 1,	5.4	5
570	Optical properties of silicene, Si/Ag(111), and Si/Ag(110). *Physical Review B*, **2018**, 97,	3.3	21
569	Correlation beyond the random phase approximation: A consistent many-body perturbation theory approach. *Physical Review B*, **2018**, 97,	3.3	3
568	Optical Properties of Silicene and Related Materials from First Principles. *Nanoscience and Technology*, **2018**, 73-98	0.6	3
567	Strong in- and out-of-plane excitons in two-dimensional InN nanosheets. *Physical Review B*, **2018**, 98,	3.3	21
566	Ab initio optical and energy loss spectra of transition metal monopnictides TaAs, TaP, NbAs, and NbP. *Journal of Applied Physics*, **2018**, 124, 205110	2.5	5
565	Vibrational properties of GaSe: a layer dependent study from experiments to theory. *Semiconductor Science and Technology*, **2018**, 33, 125008	1.8	6
564	Spontaneous symmetry breaking and electronic and dielectric properties in commensurate La7/4Sr1/4CuO4 and La5/3Sr1/3NiO4. *Physical Review B*, **2018**, 97,	3.3	3
563	Tunable electronic properties of two-dimensional nitrides for light harvesting heterostructures. *Applied Physics Letters*, **2017**, 110, 012103	3.4	44
562	Tuning Electronic Properties and Band Alignments of Phosphorene Combined With MoSe2 and WSe2. *Journal of Physical Chemistry C*, **2017**, 121, 3862-3869	3.8	42
561	Fast and accurate approximate quasiparticle band structure calculations of ZnO, CdO, and MgO polymorphs. *Physical Review B*, **2017**, 95,	3.3	18
560	Electronic and optical properties of topological semimetal CdAs. *Scientific Reports*, **2017**, 7, 45500	4.9	27

559	Optical absorbance and band-gap engineering of (BN)1⊠(C2)x two-dimensional alloys: Phase separation and composition fluctuation effects. *Physical Review B*, **2017**, 95,	3.3	19
558	Deposition of topological silicene, germanene and stanene on graphene-covered SiC substrates. *Scientific Reports*, **2017**, 7, 15700	4.9	27
557	Chemically Tunable Properties of Graphene Covered Simultaneously with Hydroxyl and Epoxy Groups. *Journal of Physical Chemistry C*, **2017**, 121, 27603-27611	3.8	4
556	Critical Temperature for the Conversion from Wurtzite to Zincblende of the Optical Emission of InAs Nanowires. *Journal of Physical Chemistry C*, **2017**, 121, 16650-16656	3.8	0
555	Thermodynamic, electronic, and optical properties of graphene oxide: A statistical ab initio approach. *Physical Review B*, **2017**, 95,	3.3	14
554	Coincidence Lattices and Interlayer Twist in van der Waals Heterostructures: Application of the Coincidence Lattice Method on (hbox {hBN/MoSe}_2) Heterobilayer Systems. *Journal of Electronic Materials*, **2017**, 46, 3910-3916	1.9	7
553	Ferroelectric phase transition in multiferroic Ge Mn Te driven by local lattice distortions. *Physical Review B*, **2016**, 94,	3.3	11
552	Intrinsic spin Hall conductivity in one-, two-, and three-dimensional trivial and topological systems. *Physical Review B*, **2016**, 94,	3.3	13
551	Quantum spin Hall effect in ⊠n/CdTe(001) quantum-well structures. *Physical Review B*, **2016**, 93,	3.3	5
550	Quasiparticle bands and spectra of Ga2O3 polymorphs. *Physical Review B*, **2016**, 93,	3.3	117
549	Atomic configurations of Au-induced nanowires on Ge(001) stabilized by higher Au coverages. *Physical Review B*, **2016**, 93,	3.3	7
548	Quantization and topological states in the spin Hall conductivity of low-dimensional systems: An ab initio study. *Physical Review B*, **2016**, 93,	3.3	8
547	Influence of out-of-plane response on optical properties of two-dimensional materials: First principles approach. *Physical Review B*, **2016**, 94,	3.3	48
546	Half-Heusler compounds with a 1 eV (1.7 eV) direct band gap, lattice-matched to GaAs (Si), for solar cell application: A first-principles study. *Physica Status Solidi (B): Basic Research*, **2016**, 253, 889-894	1.3	9
545	Pseudodirect to Direct Compositional Crossover in Wurtzite GaP/InGaP Core-Shell Nanowires. *Nano Letters*, **2016**, 16, 7930-7936	11.5	17
544	Optical study of the band structure of wurtzite GaP nanowires. *Journal of Applied Physics*, **2016**, 120, 044304	2.5	28
543	Hund's Rule-Driven Dzyaloshinskii-Moriya Interaction at 3d-5d Interfaces. *Physical Review Letters*, **2016**, 117, 247202	7.4	105
542	Quantum spin Hall phase in stanene-derived overlayers on passivated SiC substrates. *Physical Review B*, **2016**, 94,	3.3	14

541	Coverage-dependent geometries of nanowires on Ge(0 0 1)-Au surfaces: modification of trenches. *Journal of Physics Condensed Matter*, **2016**, 28, 284005	1.8	3
540	Influence of the composition fluctuations and decomposition on the tunable direct gap and oscillator strength of Ge1-xSnx alloys. *Applied Physics Letters*, **2016**, 108, 092101	3.4	17
539	Flexible 2D Crystals of Polycyclic Aromatics Stabilized by Static Distortion Waves. *ACS Nano*, **2016**, 10, 6474-83	16.7	17
538	Coincidence Lattices of 2D Crystals: Heterostructure Predictions and Applications. *Journal of Physical Chemistry C*, **2016**, 120, 10895-10908	3.8	51
537	Optical Properties of Strained Wurtzite Gallium Phosphide Nanowires. *Nano Letters*, **2016**, 16, 3703-9	11.5	34
536	Dipole analysis of the dielectric function of color dispersive materials: Application to monoclinic Ga2O3. *Physical Review B*, **2016**, 94,	3.3	44
535	Stability and electronic structure of two-dimensional allotropes of group-IV materials. *Physical Review B*, **2015**, 92,	3.3	98
534	Model GW Studies. *Springer Series in Solid-state Sciences*, **2015**, 327-350	0.4	
533	Energies and Forces. *Springer Series in Solid-state Sciences*, **2015**, 129-161	0.4	
532	Metal-to-Insulator Transition in Au Chains on Si(111)-5□-Au by Band Filling: Infrared Plasmonic Signal and Ab Initio Band Structure Calculation. *Journal of Physical Chemistry Letters*, **2015**, 6, 3615-20	6.4	12
531	Many-Body Approach to Electronic Excitations. *Springer Series in Solid-state Sciences*, **2015**,	0.4	79
530	Excitons in two-dimensional sheets with honeycomb symmetry. *Physica Status Solidi (B): Basic Research*, **2015**, 252, 72-77	1.3	18
529	Wurtzite silicon as a potential absorber in photovoltaics: Tailoring the optical absorption by applying strain. *Physical Review B*, **2015**, 92,	3.3	39
528	Influence of structure and thermodynamic stability on electronic properties of two-dimensional SiC, SiGe, and GeC alloys. *Physical Review B*, **2015**, 92,	3.3	41
527	Spin-dependent properties and images of MnO, FeO, CoO, and NiO(001) surfaces. *Physical Review B* , **2015**, 92,	3.3	10
526	Near valence-band electronic properties of semiconducting □Ga2O3 (100) single crystals. *Physical Review B*, **2015**, 92,	3.3	27
525	Dielectric tensor of monoclinic Ga2O3 single crystals in the spectral range 0.5□8.5 eV. *APL Materials* , **2015**, 3, 106106	5.7	65
524	Metallic Properties of the Si(111) - 5 □ - Au Surface from Infrared Plasmon Polaritons and Ab Initio Theory. *Nano Letters*, **2015**, 15, 4155-60	11.5	23

523	Amorphous Ge quantum dots embedded in crystalline Si: ab initio results. *Journal of Physics Condensed Matter*, **2015**, 27, 405302	1.8	7
522	Hamiltonian of Interacting Electrons. *Springer Series in Solid-state Sciences*, **2015**, 13-27	0.4	
521	Topological states in Sn and HgTe quantum wells: A comparison of ab initio results. *Physical Review B*, **2015**, 91,	3.3	17
520	Density Correlation and Electronic Polarization. *Springer Series in Solid-state Sciences*, **2015**, 255-286	0.4	
519	Kohn-Sham Scheme. *Springer Series in Solid-state Sciences*, **2015**, 89-104	0.4	
518	Electron-Hole Problem. *Springer Series in Solid-state Sciences*, **2015**, 439-457	0.4	
517	Beyond Static Screening. *Springer Series in Solid-state Sciences*, **2015**, 539-572	0.4	
516	Non-local Exchange and Correlation. *Springer Series in Solid-state Sciences*, **2015**, 163-195	0.4	
515	Si(111)2 1 surface isomers: DFT investigations on stability and doping effects. *Surface Science*, **2014**, 621, 123-127	1.8	4
514	Silicene-derived phases on Ag(111) substrate versus coverage: Ab initio studies. *Physical Review B*, **2014**, 89,	3.3	54
513	Unexpected symmetry and AA stacking of bilayer silicene on Ag(111). *Physical Review B*, **2014**, 89,	3.3	24
512	Topological Sn surface states versus film thickness and strain. *Physical Review B*, **2014**, 90,	3.3	23
511	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
510	One- and two-particle effects in the electronic and optical spectra of barium fluoride. *Journal of Physics Condensed Matter*, **2014**, 26, 125501	1.8	3
509	Polytypism in ZnS, ZnSe, and ZnTe: First-principles study. *Physical Review B*, **2014**, 89,	3.3	31
508	Nonmetallic substrates for growth of silicene: an ab initio prediction. *Journal of Physics Condensed Matter*, **2014**, 26, 185002	1.8	41
507	Silicene on metal and metallized surfaces:ab initiostudies. *New Journal of Physics*, **2014**, 16, 075004	2.9	24
506	Magnetic exchange force microscopy from first principles: application to the antiferromagnetic NiO(001) surface. *New Journal of Physics*, **2014**, 16, 023020	2.9	7

505	Influence of edge and field effects on topological states of germanene nanoribbons from self-consistent calculations. *Physical Review B*, **2014**, 90,	3.3	39
504	Topological transition and edge states in HgTe quantum wells from first principles. *Physical Review B*, **2014**, 89,	3.3	13
503	First-principles calculations of energetics and electronic structure for reconstructed Si(111)(5□)Au surfaces. *Physical Review B*, **2014**, 90,	3.3	8
502	Structural and Magnetic Properties of MnTe Phases from Ab Initio Calculations. *Journal of Superconductivity and Novel Magnetism*, **2013**, 26, 1963-1972	1.5	21
501	Silicene on hydrogen-passivated Si(111) and Ge(111) substrates. *Physica Status Solidi - Rapid Research Letters*, **2013**, 7, 538-541	2.5	29
500	Universal infrared absorbance of two-dimensional honeycomb group-IV crystals. *Physical Review B*, **2013**, 87,	3.3	122
499	Structure, energetics, and electronic states of III-V compound polytypes. *Journal of Physics Condensed Matter*, **2013**, 25, 273201	1.8	80
498	Effects of strain on the valence band structure and exciton-polariton energies in ZnO. *Physical Review B*, **2013**, 88,	3.3	31
497	Massive Dirac quasiparticles in the optical absorbance of graphene, silicene, germanene, and tinene. *Journal of Physics Condensed Matter*, **2013**, 25, 395305	1.8	134
496	Structural and electronic properties of □tin nanocrystals from first principles. *Physical Review B*, **2013**, 87,	3.3	24
495	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
494	Relation between spontaneous polarization and crystal field from first principles. *Physical Review B*, **2013**, 87,	3.3	33
493	Theoretical optical spectroscopy of complex systems. *Journal of Electron Spectroscopy and Related Phenomena*, **2013**, 189, 46-55	1.7	7
492	Enhanced Optical Absorption Due to Symmetry Breaking in TiO2(1□)S2x Alloys. *Journal of Physical Chemistry C*, **2013**, 117, 4189-4193	3.8	13
491	Electronic and optical properties of cadmium fluoride: The role of many-body effects. *Physical Review B*, **2013**, 87,	3.3	13
490	Ab initio calculation of optical properties with excitonic effects in wurtzite InxGa1□N and InxAl1□N alloys. *Physical Review B*, **2013**, 87,	3.3	13
489	Direct band gap wurtzite gallium phosphide nanowires. *Nano Letters*, **2013**, 13, 1559-63	11.5	230
488	Unit cell structure of the wurtzite phase of GaP nanowires: X-ray diffraction studies and density functional theory calculations. *Physical Review B*, **2013**, 88,	3.3	27

487	Magnetic anisotropy of FeO and CoO: the influence of gradient corrections on exchange and correlation. *Journal of Physics Condensed Matter*, **2013**, 25, 486002	1.8	6
486	Optical absorption and emission of Sn nanocrystals from first principles. *Nanotechnology*, **2013**, 24, 405702	3.4	10
485	Electronic Surface Properties of Transparent Conducting Oxides: An Ab Initio Study **2013**, 119-128		
484	Influence of on-site Coulomb interaction U on properties of MnO(001)2 1 and NiO(001)2 1 surfaces. *Journal of Physics Condensed Matter*, **2013**, 25, 094006	1.8	9
483	Magnetic exchange forces and d-state filling: Antiferromagnetic MnO(001) and NiO(001) surfaces. *Physical Review B*, **2013**, 88,	3.3	3
482	In4d and Ga3d levels in InxX1 N (X = Ga, Al) alloys. *Applied Physics Letters*, **2013**, 102, 172105	3.4	1
481	Ab-initio study of Mg-doped InN(0001) surface. *AIP Advances*, **2013**, 3, 012102	1.5	2
480	Ab initio investigation of graphene-based one-dimensional superlattices and their interfaces. *Physical Review B*, **2012**, 86,	3.3	13
479	Direct experimental determination of the spontaneous polarization of GaN. *Physical Review B*, **2012** , 86,	3.3	82
478	Geometric, electronic, and optical properties of the Si(111)2 1 surface: Positive and negative buckling. *Physical Review B*, **2012**, 86,	3.3	14
477	Electronic bands of III-V semiconductor polytypes and their alignment. *Physical Review B*, **2012**, 86,	3.3	126
476	Influence of separation of Si nanocrystals embedded in a SiO2 matrix on electronic and optical properties. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **2012**, 177, 1098-1102	3.1	4
475	Structural, electrical, and optical properties of hydrogen-doped ZnO films. *Physical Review B*, **2012**, 86,	3.3	37
474	Crystalline and magnetic anisotropy of the 3d-transition metal monoxides MnO, FeO, CoO, and NiO. *Physical Review B*, **2012**, 86,	3.3	77
473	Optical and energy-loss spectra of the antiferromagnetic transition metal oxides MnO, FeO, CoO, and NiO including quasiparticle and excitonic effects. *Physical Review B*, **2012**, 86,	3.3	51
472	Distribution of cations in wurtzitic InxGa1 N and InxAl1 N alloys: Consequences for energetics and quasiparticle electronic structures. *Physical Review B*, **2012**, 85,	3.3	18
471	Beyond the GW approximation: Combining correlation channels. *Physical Review B*, **2012**, 85,	3.3	52
470	First-principles optical spectra for F centers in MgO. *Physical Review Letters*, **2012**, 108, 126404	7.4	131

469	Clustering of N impurities in ZnO. *Applied Physics Letters*, **2012**, 100, 022107	3.4	15
468	Infrared absorbance of silicene and germanene. *Applied Physics Letters*, **2012**, 100, 261906	3.4	134
467	Strong excitons in novel two-dimensional crystals: Silicane and germanane. *Europhysics Letters*, **2012**, 98, 37004	1.6	100
466	Tunneling of electrons between Si nanocrystals embedded in a SiO2 matrix. *Physical Review B*, **2012** , 86,	3.3	26
465	Surface Properties of Transparent Conducting Oxides from First Principles: In2O3, SnO2, and ZnO. *E-Journal of Surface Science and Nanotechnology*, **2012**, 10, 216-220	0.7	2
464	Defect induced modification of the surface gap and optical properties of C(111)2 □1 surface. *Physica Status Solidi (A) Applications and Materials Science*, **2012**, 209, 669-674	1.6	3
463	Side-dependent electron escape from graphene- and graphane-like SiC layers. *Applied Physics Letters*, **2012**, 100, 043110	3.4	35
462	Real-structure effects: Absorption edge of MgxZn1-xO, CdxZn1-xO, and n-type ZnO from ab-initio calculations **2012**,		5
461	Large bandwidths in synthetic one-dimensional stacks of biological molecules. *Physical Review B*, **2012**, 86,	3.3	7
460	Energetics and approximate quasiparticle electronic structure of low-index surfaces of SnO2. *Physical Review B*, **2012**, 86,	3.3	27
459	Structural examination of Au/Ge(001) by surface x-ray diffraction and scanning tunneling microscopy. *Physical Review B*, **2012**, 85,	3.3	15
458	Band discontinuities at Si-TCO interfaces from quasiparticle calculations: Comparison of two alignment approaches. *Physical Review B*, **2012**, 85,	3.3	56
457	Ab initio description of quasiparticle band structures and optical near-edge absorption of transparent conducting oxides. *Journal of Materials Research*, **2012**, 27, 2180-2189	2.5	23
456	Cysteine on Gold: An ab-initio Investigation **2012**, 105-117		
455	Tin dioxide from first principles: Quasiparticle electronic states and optical properties. *Physical Review B*, **2011**, 83,	3.3	129
454	Electronic and optical properties of MgxZn1□O and CdxZn1□O fromab initiocalculations. *New Journal of Physics*, **2011**, 13, 085012	2.9	49
453	Cubic inclusions in hexagonal AlN, GaN, and InN: Electronic states. *Physical Review B*, **2011**, 84,	3.3	44
452	Polytypism of GaAs, InP, InAs, and InSb: An ab initio study. *Physical Review B*, **2011**, 84,	3.3	40

451	Unit cell structure of crystal polytypes in InAs and InSb nanowires. *Nano Letters*, **2011**, 11, 1483-9	11.5	110
450	Optical absorption in degenerately doped semiconductors: Mott transition or Mahan excitons?. *Physical Review Letters*, **2011**, 107, 236405	7.4	49
449	Luminescence and absorption in germanium and silicon nanocrystals: The influence of compression, surface reconstruction, optical excitation, and spin-orbit splitting. *Physical Review B*, **2011**, 83,	3.3	15
448	Charge transport in organic crystals: Theory and modelling. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 511-525	1.3	118
447	Influence of exchange and correlation on structural and electronic properties of AlN, GaN, and InN polytypes. *Physical Review B*, **2011**, 84,	3.3	79
446	Effective density of states and carrier masses for Si/SiO2superlattices from first principles. *Semiconductor Science and Technology*, **2011**, 26, 014024	1.8	7
445	Interplay of excitonic effects and van Hove singularities in optical spectra: CaO and AlN polymorphs. *Physical Review B*, **2011**, 84,	3.3	44
444	Screening and band structure effects on quasi-one-dimensional transport in periodically modulated graphene. *Physical Review B*, **2011**, 84,	3.3	4
443	Electronic properties of polar and nonpolar InN surfaces: A quasiparticle picture. *Physical Review B*, **2011**, 84,	3.3	34
442	Ab initiocharacterization of the electronic properties of PbTe quantum dots embedded in a CdTe matrix. *Semiconductor Science and Technology*, **2011**, 26, 014005	1.8	6
441	Ab-initio Characterization of Electronic Properties of PbTe Quantum Dots Embedded in a CdTe Matrix **2011**, 135-147		
440	Organic-Metal Interface: Adsorption of Cysteine on Au(110) from First Principles **2011**, 119-134		
439	Magnetic interaction in pairwise Mn-doped Si nanocrystals. *Physical Review B*, **2010**, 82,	3.3	8
438	Valence-band splittings in cubic and hexagonal AlN, GaN, and InN. *Applied Physics Letters*, **2010**, 97, 232101	3.4	26
437	Single cysteine adsorption on Au(110): A first-principles study. *Physical Review B*, **2010**, 81,	3.3	41
436	First-principles studies of Au-induced nanowires on Ge(001). *Physical Review B*, **2010**, 81,	3.3	34
435	Charge transport in organic crystals: interplay of band transport, hopping and electron–phonon scattering. *New Journal of Physics*, **2010**, 12, 023011	2.9	57
434	Ab initio description of heterostructural alloys: Thermodynamic and structural properties of MgxZn1−xO and CdxZn1−xO. *Physical Review B*, **2010**, 81,	3.3	42

433	Influence of Strong Electron Correlation on Magnetism in Transition-Metal Doped Si Nanocrystals. *Journal of Chemical Theory and Computation*, **2010**, 6, 353-8	6.4	10
432	Band alignment at a nonplanar Si/SiO2 interface. *Physical Review B*, **2010**, 82,	3.3	28
431	Characteristics of small- and large-polaron motion in organic crystals. *Journal of Physics Condensed Matter*, **2010**, 22, 465802	1.8	10
430	Free-carrier absorption in nitrides from first principles. *Physical Review B*, **2010**, 81,	3.3	97
429	Band lineup between silicon and transparent conducting oxides. *Applied Physics Letters*, **2010**, 97, 032116	3.4	44
428	Energetic stability and magnetic properties of MnO in the rocksalt, wurtzite, and zinc-blende structures: Influence of exchange and correlation. *Physical Review B*, **2010**, 82,	3.3	52
427	Finite-size modelling of electrodes for quantum transport calculations using k-space ab initio techniques. *Computer Physics Communications*, **2010**, 181, 746-749	4.2	3
426	Electronic and transport properties of graphene nanoribbons. *Physica Status Solidi (A) Applications and Materials Science*, **2010**, 207, 304-308	1.6	28
425	Electronic and optical properties of group IV two-dimensional materials. *Physica Status Solidi (A) Applications and Materials Science*, **2010**, 207, 291-299	1.6	19
424	Spectral properties of InN and its native oxide from first principles. *Physica Status Solidi (A) Applications and Materials Science*, **2010**, 207, 1041-1053	1.6	10
423	Metal□nsulator transition in Si(111)-(4 □1)/(8 □2)-In studied by optical spectroscopy. *Physica Status Solidi (B): Basic Research*, **2010**, 247, 2033-2039	1.3	11
422	Stability of polar semiconductor heterostructures. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2010**, 7, 244-247		
421	Optical anisotropy of Si(111)-(4 □1)/(8 □2)-In nanowires calculated from first-principles. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2010**, 7, 133-136		1
420	Interface with organic molecules: Cysteine on Au(110). *Physica Status Solidi C: Current Topics in Solid State Physics*, **2010**, 7, 149-152		10
419	Adsorption of Cysteine on the Au(110)-surface: A Density Functional Theory Study **2010**, 53-60		1
418	Nanomagnetism in Transition Metal Doped Si Nanocrystals **2010**, 541-552		
417	Ab-initio Characterization of Colloidal IV-VI Semiconductor Quantum Dots **2010**, 61-73		
416	Charge-Carrier Transport Through Guanine Crystals and Stacks **2010**, 529-540		

415	Ab initio characterization of transition-metal-doped Si nanocrystals. *Physical Review B*, **2009**, 80,	3.3	11
414	Mn and Fe doping of bulk Si: Concentration influence on electronic and magnetic properties. *Physical Review B*, **2009**, 80,	3.3	21
413	Optical spectra and microscopic structure of the oxidized Si(100) surface: Combined in situ optical experiments and first principles calculations. *Physical Review B*, **2009**, 79,	3.3	20
412	Influence of the quantum confined Stark effect on photoluminescence spectra of PbTe nanodots embedded in a CdTe matrix. *Physical Review B*, **2009**, 80,	3.3	15
411	Electronic structure of In2O3 from resonant x-ray emission spectroscopy. *Applied Physics Letters*, **2009**, 94, 022105	3.4	38
410	Optical and energy-loss spectra of MgO, ZnO, and CdO from ab initio many-body calculations. *Physical Review B*, **2009**, 80,	3.3	127
409	Coherent {001} interfaces between rocksalt and zinc-blende crystal structures. *Physical Review B*, **2009**, 79,	3.3	21
408	Low-field and high-field electron transport in zinc blende InN. *Applied Physics Letters*, **2009**, 94, 022102	3.4	33
407	Structure of si(111)-in nanowires determined from the midinfrared optical response. *Physical Review Letters*, **2009**, 102, 226805	7.4	41
406	Influence of SiO2 matrix on electronic and optical properties of Si nanocrystals. *Nanotechnology*, **2009**, 20, 135702	3.4	57
405	Self-organized atomic nanowires of noble metals on Ge(001): atomic structure and electronic properties. *New Journal of Physics*, **2009**, 11, 125011	2.9	33
404	Efficiency limits of Si/SiO2 quantum well solar cells from first-principles calculations. *Journal of Applied Physics*, **2009**, 105, 104511	2.5	35
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