Alexander Zunger

List of Publications by Citations

652 papers	74,981 citations	126 h-index	255 g-index
677 ext. papers	80,081 ext. citations	5.1 avg, IF	8.25 L-index

#	Paper	IF	Citations
652	Self-interaction correction to density-functional approximations for many-electron systems. *Physical Review B*, **1981**, 23, 5048-5079	3.3	16702
651	Special quasirandom structures. *Physical Review Letters*, **1990**, 65, 353-356	7.4	2054
650	Intrinsic n-type versus p-type doping asymmetry and the defect physics of ZnO. *Physical Review B*, **2001**, 63,	3.3	1502
649	Defect physics of the CuInSe2 chalcopyrite semiconductor. *Physical Review B*, **1998**, 57, 9642-9656	3.3	1128
648	Assessment of correction methods for the band-gap problem and for finite-size effects in supercell defect calculations: Case studies for ZnO and GaAs. *Physical Review B*, **2008**, 78,	3.3	896
647	Zinc-blende-wurtzite polytypism in semiconductors. *Physical Review B*, **1992**, 46, 10086-10097	3.3	853
646	Theory of the band-gap anomaly in ABC2 chalcopyrite semiconductors. *Physical Review B*, **1984**, 29, 1882-1906	3.3	812
645	Origins of coexistence of conductivity and transparency in SnO(2). *Physical Review Letters*, **2002**, 88, 095501	7.4	722
644	Electronic properties of random alloys: Special quasirandom structures. *Physical Review B*, **1990**, 42, 9622-9649	3.3	688
643	Calculated natural band offsets of all II–VI and III–V semiconductors: Chemical trends and the role of cation d orbitals. *Applied Physics Letters*, **1998**, 72, 2011-2013	3.4	653
642	Dopability, intrinsic conductivity, and nonstoichiometry of transparent conducting oxides. *Physical Review Letters*, **2007**, 98, 045501	7.4	543
641	Role of metal d states in II-VI semiconductors. *Physical Review B*, **1988**, 37, 8958-8981	3.3	526
640	Anion vacancies as a source of persistent photoconductivity in II-VI and chalcopyrite semiconductors. *Physical Review B*, **2005**, 72,	3.3	495
639	Predicted band-gap pressure coefficients of all diamond and zinc-blende semiconductors: Chemical trends. *Physical Review B*, **1999**, 60, 5404-5411	3.3	480
638	Giant and composition-dependent optical bowing coefficient in GaAsN alloys. *Physical Review Letters*, **1996**, 76, 664-667	7.4	478
637	Solving Schrödinger's equation around a desired energy: Application to silicon quantum dots. *Journal of Chemical Physics*, **1994**, 100, 2394-2397	3.9	459
636	Electronic structure of the ternary chalcopyrite semiconductors CuAlS2, CuGaS2, CuInS2, CuAlSe2, CuGaSe2, and CuInSe2. *Physical Review B*, **1983**, 28, 5822-5847	3.3	451

635	Effects of Ga addition to CuInSe2 on its electronic, structural, and defect properties. *Applied Physics Letters*, **1998**, 72, 3199-3201	3.4	420
634	Origins of the p-type nature and cation deficiency in Cu2O and related materials. *Physical Review B*, **2007**, 76,	3.3	402
633	Band offsets and optical bowings of chalcopyrites and Zn-based II-VI alloys. *Journal of Applied Physics*, **1995**, 78, 3846-3856	2.5	398
632	Bond lengths around isovalent impurities and in semiconductor solid solutions. *Physical Review B*, **1984**, 30, 6217-6220	3.3	395
631	n-type doping of CuInSe2 and CuGaSe2. *Physical Review B*, **2005**, 72,	3.3	384
630	Electronic structure of ZnS, ZnSe, ZnTe, and their pseudobinary alloys. *Physical Review B*, **1987**, 36, 3199-3228	3.3	378
629	Pseudopotential calculations of nanoscale CdSe quantum dots. *Physical Review B*, **1996**, 53, 9579-9582	3.3	377
628	A phenomenological model for systematization and prediction of doping limits in II-VI and I-III-VI2 compounds. *Journal of Applied Physics*, **1998**, 83, 3192-3196	2.5	372
627	Theory of electronic structure evolution in GaAsN and GaPN alloys. *Physical Review B*, **2001**, 64,	3.3	361
626	First-principles calculation of band offsets, optical bowings, and defects in CdS, CdSe, CdTe, and their alloys. *Journal of Applied Physics*, **2000**, 87, 1304-1311	2.5	360
625	Correcting density functional theory for accurate predictions of compound enthalpies of formation: Fitted elemental-phase reference energies. *Physical Review B*, **2012**, 85,	3.3	358
624	Electronic Structure Pseudopotential Calculations of Large (.apprx.1000 Atoms) Si Quantum Dots. *The Journal of Physical Chemistry*, **1994**, 98, 2158-2165		350
623	Identification of potential photovoltaic absorbers based on first-principles spectroscopic screening of materials. *Physical Review Letters*, **2012**, 108, 068701	7.4	349
622	Atomic structure and ordering in semiconductor alloys. *Physical Review B*, **1985**, 31, 2561-2564	3.3	347
621	Switching a normal insulator into a topological insulator via electric field with application to phosphorene. *Nano Letters*, **2015**, 15, 1222-8	11.5	343
620	Practical doping principles. *Applied Physics Letters*, **2003**, 83, 57-59	3.4	327
619	Band-structure, optical properties, and defect physics of the photovoltaic semiconductor SnS. *Applied Physics Letters*, **2012**, 100, 032104	3.4	317
618	Polaronic hole localization and multiple hole binding of acceptors in oxide wide-gap semiconductors. *Physical Review B*, **2009**, 80,	3.3	309

617	Valence band splittings and band offsets of AlN, GaN, and InN. *Applied Physics Letters*, **1996**, 69, 2719-2721	3.4	303
616	Dielectric constants of silicon quantum dots. *Physical Review Letters*, **1994**, 73, 1039-1042	7.4	300
615	Theoretical interpretation of the experimental electronic structure of lens-shaped self-assembled InAs/GaAs quantum dots. *Physical Review B*, **2000**, 62, 12963-12977	3.3	297
614	Pseudopotential calculation of the excitonic fine structure of million-atom self-assembled In1−xGaxAs/GaAs quantum dots. *Physical Review B*, **2003**, 67,	3.3	293
613	Hidden spin polarization in inversion-symmetric bulk crystals. *Nature Physics*, **2014**, 10, 387-393	16.2	290
612	Effects of Na on the electrical and structural properties of CuInSe2. *Journal of Applied Physics*, **1999**, 85, 7214-7218	2.5	283
611	Anomalous grain boundary physics in polycrystalline CuInSe2: the existence of a hole barrier. *Physical Review Letters*, **2003**, 91, 266401	7.4	280
610	Prediction and accelerated laboratory discovery of previously unknown 18-electron ABX compounds. *Nature Chemistry*, **2015**, 7, 308-16	17.6	276
609	First-principles statistical mechanics of structural stability of intermetallic compounds. *Physical Review B*, **1991**, 44, 512-544	3.3	274
608	Electronic structures of [110]-faceted self-assembled pyramidal InAs/GaAs quantum dots. *Physical Review B*, **1999**, 59, 5678-5687	3.3	269
607	Stabilization of Ternary Compounds via Ordered Arrays of Defect Pairs. *Physical Review Letters*, **1997**, 78, 4059-4062	7.4	264
606	Accurate prediction of defect properties in density functional supercell calculations. *Modelling and Simulation in Materials Science and Engineering*, **2009**, 17, 084002	2	263
605	Electronic and structural anomalies in lead chalcogenides. *Physical Review B*, **1997**, 55, 13605-13610	3.3	259
604	n-type doping of oxides by hydrogen. *Applied Physics Letters*, **2002**, 81, 73-75	3.4	259
603	Light- and bias-induced metastabilities in Cu(In,Ga)Se2 based solar cells caused by the (VSe-VCu) vacancy complex. *Journal of Applied Physics*, **2006**, 100, 113725	2.5	252
602	Inverse Design of High Absorption Thin-Film Photovoltaic Materials. *Advanced Energy Materials*, **2013**, 3, 43-48	21.8	251
601	Cu-Au, Ag-Au, Cu-Ag, and Ni-Au intermetallics: First-principles study of temperature-composition phase diagrams and structures. *Physical Review B*, **1998**, 57, 6427-6443	3.3	249
600	Evolutionary approach for determining first-principles hamiltonians. *Nature Materials*, **2005**, 4, 391-4	27	249

599	Localization and percolation in semiconductor alloys: GaAsN vs GaAsP. *Physical Review B*, **1996**, 54, 17568-17576	3.3	249
598	Efficient cluster expansion for substitutional systems. *Physical Review B*, **1992**, 46, 12587-12605	3.3	248
597	First-principles calculation of alloy phase diagrams: The renormalized-interaction approach. *Physical Review B*, **1989**, 40, 3197-3231	3.3	244
596	Systematization of the stable crystal structure of all AB-type binary compounds: A pseudopotential orbital-radii approach. *Physical Review B*, **1980**, 22, 5839-5872	3.3	235
595	Evolution of III-V nitride alloy electronic structure: the localized to delocalized transition. *Physical Review Letters*, **2001**, 86, 2613-6	7.4	234
594	Many-electron multiplet effects in the spectra of 3d impurities in heteropolar semiconductors. *Physical Review B*, **1984**, 30, 3430-3455	3.3	233
593	Cluster-doping approach for wide-gap semiconductors: the case of p-type ZnO. *Physical Review Letters*, **2003**, 90, 256401	7.4	232
592	First-principles calculation of temperature-composition phase diagrams of semiconductor alloys. *Physical Review B*, **1990**, 41, 8240-8269	3.3	232
591	Total-energy and band-structure calculations for the semimagnetic Cd1-xMnxTe semiconductor alloy and its binary constituents. *Physical Review B*, **1987**, 35, 2340-2365	3.3	229
590	A universal trend in the binding energies of deep impurities in semiconductors. *Applied Physics Letters*, **1984**, 45, 671-673	3.4	229
589	Direct Pseudopotential Calculation of Exciton Coulomb and Exchange Energies in Semiconductor Quantum Dots. *Physical Review Letters*, **1997**, 78, 915-918	7.4	227
588	Spatial correlations in GaInAsN alloys and their effects on band-gap enhancement and electron localization. *Physical Review Letters*, **2001**, 86, 2609-12	7.4	227
587	Cu-In Halide Perovskite Solar Absorbers. *Journal of the American Chemical Society*, **2017**, 139, 6718-6725	16.4	226
586	Extracting E versus k effective band structure from supercell calculations on alloys and impurities. *Physical Review B*, **2012**, 85,	3.3	226
585	Stability of ordered bulk and epitaxial semiconductor alloys. *Physical Review Letters*, **1986**, 56, 1400-1403	7.4	224
584	Pseudopotential theory of Auger processes in CdSe quantum dots. *Physical Review Letters*, **2003**, 91, 056404	7.4	223
583	The inverse band-structure problem of finding an atomic configuration with given electronic properties. *Nature*, **1999**, 402, 60-63	50.4	221
582	First-Principles Prediction of Vacancy Order-Disorder and Intercalation Battery Voltages in LixCoO2. *Physical Review Letters*, **1998**, 81, 606-609	7.4	217

581	Band gaps and spin-orbit splitting of ordered and disordered AlxGa1-xAs and GaAsxSb1-x alloys. *Physical Review B*, **1989**, 39, 3279-3304	3.3	217
580	InP quantum dots: Electronic structure, surface effects, and the redshifted emission. *Physical Review B*, **1997**, 56, 1496-1508	3.3	216
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578	A polarity-induced defect mechanism for conductivity and magnetism at polar-nonpolar oxide interfaces. *Nature Communications*, **2014**, 5, 5118	17.4	209
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576	Localization and anticrossing of electron levels in GaAs1□Nx alloys. *Physical Review B*, **1999**, 60, R11245-R11248	3.3	197
575	Assessing capability of semiconductors to split water using ionization potentials and electron affinities only. *Physical Chemistry Chemical Physics*, **2014**, 16, 3706-14	3.6	194
574	Band structure and lattice instability of TiSe2. *Physical Review B*, **1978**, 17, 1839-1842	3.3	192
573	Electronic Structure of 3d Transition-Atom Impurities in Semiconductors. *Solid State Physics*, **1986**, 39, 275-464	2	188
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571	Ground- and excited-state properties of LiF in the local-density formalism. *Physical Review B*, **1977**, 16, 2901-2926	3.3	185
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568	Origins of the doping asymmetry in oxides: Hole doping in NiO versus electron doping in ZnO. *Physical Review B*, **2007**, 75,	3.3	182
567	Long-Range Spin Currents with Chiral Crystals. *Physics Magazine*, **2010**, 3,	1.1	180
566	Microscopic origin of the phenomenological equilibrium "Doping limit Rule" in n-type III-V semiconductors. *Physical Review Letters*, **2000**, 84, 1232-5	7.4	180
565	Optical bowing in zinc chalcogenide semiconductor alloys. *Physical Review B*, **1986**, 34, 5992-5995	3.3	180
564	First-principles nonlocal-pseudopotential approach in the density-functional formalism. II. Application to electronic and structural properties of solids. *Physical Review B*, **1979**, 20, 4082-4108	3.3	180

563	Structural and electronic properties of epitaxial thin-layer SinGen superlattices. *Physical Review B*, **1988**, 37, 6893-6907	3.3	179
562	First-principles nonlocal-pseudopotential approach in the density-functional formalism: Development and application to atoms. *Physical Review B*, **1978**, 18, 5449-5472	3.3	178
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560	Al on GaAs(110) interface: Possibility of adatom cluster formation. *Physical Review B*, **1981**, 24, 4372-4394	3.3	174
559	Structural Origin of Optical Bowing in Semiconductor Alloys. *Physical Review Letters*, **1983**, 51, 662-665	7.4	172
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557	Self-consistent numerical-basis-set linear-combination-of-atomic-orbitals investigation of the electronic structure and properties of TiS2. *Physical Review B*, **1977**, 16, 906-924	3.3	166
556	Temperature dependence of excitonic radiative decay in CdSe quantum dots: the role of surface hole traps. *Nano Letters*, **2005**, 5, 2360-4	11.5	162
555	Resonant hole localization and anomalous optical bowing in InGaN alloys. *Applied Physics Letters*, **1999**, 74, 1842-1844	3.4	159
554	Instilling defect tolerance in new compounds. *Nature Materials*, **2017**,	27	156
553	Inverse design in search of materials with target functionalities. *Nature Reviews Chemistry*, **2018**, 2,	34.6	154
552	Linear combination of bulk bands method for large-scale electronic structure calculations on strained nanostructures. *Physical Review B*, **1999**, 59, 15806-15818	3.3	154
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550	New optical transitions in strained Si-Ge superlattices. *Physical Review B*, **1987**, 36, 4547-4550	3.3	151
549	New approach for solving the density-functional self-consistent-field problem. *Physical Review B*, **1982**, 26, 3114-3137	3.3	151
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547	The peculiar electronic structure of PbSe quantum dots. *Nano Letters*, **2006**, 6, 2728-35	11.5	146
546	Band gaps of GaPN and GaAsN alloys. *Applied Physics Letters*, **1997**, 70, 3558-3560	3.4	145

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543	Atomic control of conductivity versus ferromagnetism in wide-gap oxides via selective doping: V, Nb, Ta in anatase TiO2. *Physical Review Letters*, **2008**, 100, 036601	7.4	141
542	Anion displacements and the band-gap anomaly in ternary ABC2 chalcopyrite semiconductors. *Physical Review B*, **1983**, 27, 5176-5179	3.3	141
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537	Local-density-derived semiempirical pseudopotentials. *Physical Review B*, **1995**, 51, 17398-17416	3.3	137
536	Unusual directional dependence of exchange energies in GaAs diluted with Mn: is the RKKY description relevant?. *Physical Review Letters*, **2004**, 93, 177201	7.4	133
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533	Global space-group optimization problem: Finding the stablest crystal structure without constraints. *Physical Review B*, **2007**, 75,	3.3	131
532	Composition dependence of interband transition intensities in GaPN, GaAsN, and GaPAs alloys. *Physical Review B*, **1997**, 56, 10233-10240	3.3	130
531	Iron Chalcogenide Photovoltaic Absorbers. *Advanced Energy Materials*, **2011**, 1, 748-753	21.8	128
530	Magnetic interactions of Cr□r and Co□o impurity pairs in ZnO within a band-gap corrected density functional approach. *Physical Review B*, **2008**, 77,	3.3	128
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516	Cation and vacancy ordering in LixCoO2. *Physical Review B*, **1998**, 57, 2242-2252	3.3	113
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511	Electronic structure of LiZnN: Interstitial insertion rule. *Physical Review B*, **1985**, 32, 1386-1389	3.3	108
510	High-Energy Excitonic Transitions in CdSe Quantum Dots. *Journal of Physical Chemistry B*, **1998**, 102, 6449-6454	3.4	107

509	Empirical atomic pseudopotentials for AlAs/GaAs superlattices, alloys, and nanostructures. *Physical Review B*, **1994**, 50, 17393-17405	3.3	105
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507	Density-functional theory of the correlation energy in atoms and ions: A simple analytic model and a challenge. *Physical Review A*, **1981**, 23, 2785-2789	2.6	104
506	Applicability of the k?p method to the electronic structure of quantum dots. *Physical Review B*, **1998**, 57, 9971-9987	3.3	103
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498	Ordering of isovalent intersemiconductor alloys. *Physical Review B*, **1988**, 38, 6338-6341	3.3	99
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483	Sorting Stable versus Unstable Hypothetical Compounds: The Case of Multi-Functional ABX Half-Heusler Filled Tetrahedral Structures. *Advanced Functional Materials*, **2012**, 22, 1425-1435	15.6	91
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