# Alexander Zunger

## List of Publications by Year in Descending Order



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|---|---|---|---|
| 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 | Bulk NdNiO2 is thermodynamically unstable with respect to decomposition while hydrogenation reduces the instability and transforms it from metal to insulator. *Physical Review B*, **2022**, 105, | 3.3 | 7 |
| 651 | Piezoelectricity in nominally centrosymmetric phases. *Physical Review Research*, **2021**, 3, | 3.9 | 4 |
| 650 | Intrinsic doping limitations in inorganic lead halide perovskites.. *Materials Horizons*, **2021**, | 14.4 | 1 |
| 649 | Mass enhancement in 3d and sp perovskites from symmetry breaking. *Physical Review B*, **2021**, 103, | 3.3 | 6 |
| 648 | Strong influence of nonmagnetic ligands on the momentum-dependent spin splitting in antiferromagnets. *Physical Review B*, **2021**, 103, | 3.3 | 2 |
| 647 | Prediction of low-Z collinear and noncollinear antiferromagnetic compounds having momentum-dependent spin splitting even without spin-orbit coupling. *Physical Review Materials*, **2021**, 5, | 3.2 | 11 |
| 646 | Understanding Doping of Quantum Materials. *Chemical Reviews*, **2021**, 121, 3031-3060 | 68.1 | 27 |
| 645 | Effect of static local distortions vs. dynamic motions on the stability and band gaps of cubic oxide and halide perovskites. *Materials Today*, **2021**, | 21.8 | 4 |
| 644 | Different shapes of spin textures as a journey through the Brillouin zone. *Physical Review B*, **2021**, 104, | 3.3 | 3 |
| 643 | False metals, real insulators, and degenerate gapped metals. *Applied Physics Reviews*, **2020**, 7, 041310 | 17.3 | 15 |
| 642 | Understanding electronic peculiarities in tetragonal FeSe as local structural symmetry breaking. *Physical Review B*, **2020**, 102, | 3.3 | 10 |
| 641 | Hole antidoping of oxides. *Physical Review B*, **2020**, 101, | 3.3 | 6 |
| 640 | Polymorphous nature of cubic halide perovskites. *Physical Review B*, **2020**, 101, | 3.3 | 43 |
| 639 | Ferri-chiral compounds with potentially switchable Dresselhaus spin splitting. *Physical Review B*, **2020**, 102, | 3.3 | 2 |
| 638 | The Rashba Scale: Emergence of Band Anti-crossing as a Design Principle for Materials with Large Rashba Coefficient. *Matter*, **2020**, 3, 145-165 | 12.7 | 9 |
| 637 | Symmetry-breaking polymorphous descriptions for correlated materials without interelectronic U. *Physical Review B*, **2020**, 102, | 3.3 | 19 |
| 636 | Giant momentum-dependent spin splitting in centrosymmetric low-Z antiferromagnets. *Physical Review B*, **2020**, 102, | 3.3 | 25 |

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| 635 | Inverse design of compounds that have simultaneously ferroelectric and Rashba cofunctionality. *Physical Review B*, **2020**, 102, | 3.3 | 6 |
| 634 | Realization of predicted exotic materials: The burden of proof. *Materials Today*, **2020**, 32, 35-45 | 21.8 | 17 |
| 633 | Beware of plausible predictions of fantasy materials. *Nature*, **2019**, 566, 447-449 | 50.4 | 47 |
| 632 | Design of Mixed-Cation Tri-Layered Pb-Free Halide Perovskites for Optoelectronic Applications. *Advanced Electronic Materials*, **2019**, 5, 1900234 | 6.4 | 18 |
| 631 | Antidoping in Insulators and Semiconductors Having Intermediate Bands with Trapped Carriers. *Physical Review Letters*, **2019**, 122, 106403 | 7.4 | 20 |
| 630 | Origin of band gaps in 3d perovskite oxides. *Nature Communications*, **2019**, 10, 1658 | 17.4 | 76 |
| 629 | Uncovering and tailoring hidden Rashba spin-orbit splitting in centrosymmetric crystals. *Nature Communications*, **2019**, 10, 906 | 17.4 | 21 |
| 628 | Digging for topological property in disordered alloys: the emergence of Weyl semimetal phase and sequential band inversions in PbSe$_{1-x}$Sn$_x$Se alloys. *Materials Horizons*, **2019**, 6, 2124-2134 | 14.4 | 8 |
| 627 | Mott gapping in 3dABO3 perovskites without Mott-Hubbard interelectronic repulsion energy U. *Physical Review B*, **2019**, 100, | 3.3 | 34 |
| 626 | Spontaneous Non-stoichiometry and Ordering in Degenerate but Gapped Transparent Conductors. *Matter*, **2019**, 1, 280-294 | 12.7 | 17 |
| 625 | Alloy theory with atomic resolution for Rashba or topological systems. *Physical Review Materials*, **2019**, 3, | 3.2 | 2 |
| 624 | Origins versus fingerprints of the Jahn-Teller effect in d-electron ABX3 perovskites. *Physical Review Research*, **2019**, 1, | 3.9 | 13 |
| 623 | Formation and Composition-Dependent Properties of Alloys of Cubic Halide Perovskites. *Chemistry of Materials*, **2019**, 31, 2497-2506 | 9.6 | 27 |
| 622 | Polymorphous band structure model of gapping in the antiferromagnetic and paramagnetic phases of the Mott insulators MnO, FeO, CoO, and NiO. *Physical Review B*, **2018**, 97, | 3.3 | 57 |
| 621 | Inverse design in search of materials with target functionalities. *Nature Reviews Chemistry*, **2018**, 2, | 34.6 | 154 |
| 620 | Bond disproportionation, charge self-regulation, and ligand holes in sp and in d-electron ABX3 perovskites by density functional theory. *Physical Review B*, **2018**, 98, | 3.3 | 28 |
| 619 | Predictions of new ABO3 perovskite compounds by combining machine learning and density functional theory. *Physical Review Materials*, **2018**, 2, | 3.2 | 88 |
| 618 | Topological Insulators versus Topological Dirac Semimetals in Honeycomb Compounds. *Journal of the American Chemical Society*, **2018**, 140, 13687-13694 | 16.4 | 21 |

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| 617 | Electron Doping of Proposed Kagome Quantum Spin Liquid Produces Localized States in the Band Gap. *Physical Review Letters*, **2018**, 121, 186402 | 7.4 | 17 |
| 616 | Natural off-stoichiometry causes carrier doping in half-Heusler filled tetrahedral structures. *Physical Review B*, **2017**, 95, | 3.3 | 45 |
| 615 | Cu-In Halide Perovskite Solar Absorbers. *Journal of the American Chemical Society*, **2017**, 139, 6718-6725 | 16.4 | 226 |
| 614 | Functionality-Directed Screening of Pb-Free Hybrid Organic–Inorganic Perovskites with Desired Intrinsic Photovoltaic Functionalities. *Chemistry of Materials*, **2017**, 29, 524-538 | 9.6 | 110 |
| 613 | CuTaS3: Intermetal d–d Transitions Enable High Solar Absorption. *Chemistry of Materials*, **2017**, 29, 2594-2608 | 9.6 | 17 |
| 612 | Absence of redshift in the direct bandgap of silicon nanocrystals with reduced size. *Nature Nanotechnology*, **2017**, 12, 930-932 | 28.7 | 15 |
| 611 | Predicted electronic markers for polytypes of LaOBiS2 examined via angle-resolved photoemission spectroscopy. *Physical Review B*, **2017**, 95, | 3.3 | 17 |
| 610 | Rapid Transition of the Hole Rashba Effect from Strong Field Dependence to Saturation in Semiconductor Nanowires. *Physical Review Letters*, **2017**, 119, 126401 | 7.4 | 8 |
| 609 | The Enabling Electronic Motif for Topological Insulation in ABO3 Perovskites. *Advanced Functional Materials*, **2017**, 27, 1701266 | 15.6 | 17 |
| 608 | Predicted Realization of Cubic Dirac Fermion in Quasi-One-Dimensional Transition-Metal Monochalcogenides. *Physical Review X*, **2017**, 7, | 9.1 | 44 |
| 607 | Changes in charge density vs changes in formal oxidation states: The case of Sn halide perovskites and their ordered vacancy analogues. *Physical Review Materials*, **2017**, 1, | 3.2 | 34 |
| 606 | Instilling defect tolerance in new compounds. *Nature Materials*, **2017**, | 27 | 156 |
| 605 | Minimal ingredients for orbital-texture switches at Dirac points in strong spin–orbit coupled materials. *Npj Quantum Materials*, **2016**, 1, | 5 | 4 |
| 604 | Polytypism in LaOBiS2-type compounds based on different three-dimensional stacking sequences of two-dimensional BiS2 layers. *Physical Review B*, **2016**, 93, | 3.3 | 28 |
| 603 | Single-dot absorption spectroscopy and theory of silicon nanocrystals. *Physical Review B*, **2016**, 93, | 3.3 | 31 |
| 602 | Strong Absorption Enhancement in Si Nanorods. *Nano Letters*, **2016**, 16, 7937-7941 | 11.5 | 10 |
| 601 | Quasi-Direct Optical Transitions in Silicon Nanocrystals with Intensity Exceeding the Bulk. *Nano Letters*, **2016**, 16, 1583-9 | 11.5 | 52 |
| 600 | Transforming Common III–V and II–VI Semiconductor Compounds into Topological Heterostructures: The Case of CdTe/InSb Superlattices. *Advanced Functional Materials*, **2016**, 26, 3259-3267 | 15.6 | 21 |

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|---|---|---|---|
| 599 | Orbital mapping of energy bands and the truncated spin polarization in three-dimensional Rashba semiconductors. *Physical Review B*, **2016**, 94, | 3.3 | 10 |
| 598 | Intrinsic circular polarization in centrosymmetric stacks of transition-metal dichalcogenide compounds. *Physical Review Letters*, **2015**, 114, 087402 | 7.4 | 41 |
| 597 | Split Dirac cones in HgTe/CdTe quantum wells due to symmetry-enforced level anticrossing at interfaces. *Physical Review B*, **2015**, 91, | 3.3 | 57 |
| 596 | Design and discovery of a novel half-Heusler transparent hole conductor made of all-metallic heavy elements. *Nature Communications*, **2015**, 6, 7308 | 17.4 | 75 |
| 595 | Prediction and accelerated laboratory discovery of previously unknown 18-electron ABX compounds. *Nature Chemistry*, **2015**, 7, 308-16 | 17.6 | 276 |
| 594 | Prediction and Synthesis of Strain Tolerant RbCuTe Crystals Based on Rotation of One-Dimensional Nano Ribbons within a Three-Dimensional Inorganic Network. *Journal of the American Chemical Society*, **2015**, 137, 11383-90 | 16.4 | 11 |
| 593 | Research Update: Towards designed functionalities in oxide-based electronic materials. *APL Materials*, **2015**, 3, 080702 | 5.7 | 23 |
| 592 | Reinterpretation of the expected electronic density of states of semiconductor nanowires. *Nano Letters*, **2015**, 15, 88-95 | 11.5 | 8 |
| 591 | Search and design of nonmagnetic centrosymmetric layered crystals with large local spin polarization. *Physical Review B*, **2015**, 91, | 3.3 | 35 |
| 590 | Emergence of a few distinct structures from a single formal structure type during high-throughput screening for stable compounds: The case of RbCuS and RbCuSe. *Physical Review B*, **2015**, 92, | 3.3 | 9 |
| 589 | Supercoupling between heavy-hole and light-hole states in nanostructures. *Physical Review B*, **2015**, 92, | 3.3 | 24 |
| 588 | Incomplete Peierls-like chain dimerization as a mechanism for intrinsic conductivity and optical transparency: A La-Cu-O-S phase with mixed-anion layers as a case study. *Physical Review B*, **2015**, 92, | 3.3 | 2 |
| 587 | Intrinsic Transparent Conductors without Doping. *Physical Review Letters*, **2015**, 115, 176602 | 7.4 | 26 |
| 586 | Cation ordering induced polarization enhancement for PbTiO3–SrTiO3 ferroelectric-dielectric superlattices. *Physical Review B*, **2015**, 91, | 3.3 | 5 |
| 585 | Switching a normal insulator into a topological insulator via electric field with application to phosphorene. *Nano Letters*, **2015**, 15, 1222-8 | 11.5 | 343 |
| 584 | Evolution of electronic structure as a function of layer thickness in group-VIB transition metal dichalcogenides: emergence of localization prototypes. *Nano Letters*, **2015**, 15, 949-57 | 11.5 | 57 |
| 583 | Hidden spin polarization in inversion-symmetric bulk crystals. *Nature Physics*, **2014**, 10, 387-393 | 16.2 | 290 |
| 582 | 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 |

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|---|---|---|---|
| 581 | Structurally unstable AIIIBiO3 perovskites are predicted to be topological insulators but their stable structural forms are trivial band insulators. *Physical Review B*, **2014**, 90, | 3.3 | 19 |
| 580 | A polarity-induced defect mechanism for conductivity and magnetism at polar-nonpolar oxide interfaces. *Nature Communications*, **2014**, 5, 5118 | 17.4 | 209 |
| 579 | Self-Doping and Electrical Conductivity in Spinel Oxides: Experimental Validation of Doping Rules. *Chemistry of Materials*, **2014**, 26, 1867-1873 | 9.6 | 31 |
| 578 | 2D optical photon echo spectroscopy of a self-assembled quantum dot. *Annalen Der Physik*, **2013**, 525, 31-42 | 2.6 | 9 |
| 577 | Crystal structures and metastability of carbon-boron compounds C3B and C5B. *Physical Review B*, **2013**, 87, | 3.3 | 20 |
| 576 | Li-Doped Cr2MnO4: A New p-Type Transparent Conducting Oxide by Computational Materials Design. *Advanced Functional Materials*, **2013**, 23, 5267-5276 | 15.6 | 50 |
| 575 | Theoretical prediction and experimental realization of new stable inorganic materials using the inverse design approach. *Journal of the American Chemical Society*, **2013**, 135, 10048-54 | 16.4 | 95 |
| 574 | Inverse Design of High Absorption Thin-Film Photovoltaic Materials. *Advanced Energy Materials*, **2013**, 3, 43-48 | 21.8 | 251 |
| 573 | Genetic design of enhanced valley splitting towards a spin qubit in silicon. *Nature Communications*, **2013**, 4, 2396 | 17.4 | 32 |
| 572 | Co3O4□Co2ZnO4 spinels: The case for a solid solution. *Journal of Solid State Chemistry*, **2012**, 190, 143-149 | 3.3 | 13 |
| 571 | Three-dimensional assemblies of semiconductor quantum dots in a wide-gap matrix providing an intermediate band for absorption. *Journal of Applied Physics*, **2012**, 112, 114320 | 2.5 | 8 |
| 570 | Extracting E versus k effective band structure from supercell calculations on alloys and impurities. *Physical Review B*, **2012**, 85, | 3.3 | 226 |
| 569 | 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 |
| 568 | Genomic design of strong direct-gap optical transition in Si/Ge core/multishell nanowires. *Nano Letters*, **2012**, 12, 984-91 | 11.5 | 43 |
| 567 | Band-structure, optical properties, and defect physics of the photovoltaic semiconductor SnS. *Applied Physics Letters*, **2012**, 100, 032104 | 3.4 | 317 |
| 566 | Identification of potential photovoltaic absorbers based on first-principles spectroscopic screening of materials. *Physical Review Letters*, **2012**, 108, 068701 | 7.4 | 349 |
| 565 | Angle-resolved photoemission and quasiparticle calculation of ZnO: The need for d band shift in oxide semiconductors. *Physical Review B*, **2012**, 86, | 3.3 | 49 |
| 564 | Large insulating gap in topological insulators induced by negative spin-orbit splitting. *Physical Review B*, **2012**, 86, | 3.3 | 19 |

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| 563 | Two-dimensional polaronic behavior in the binary oxides m-HfO2 and m-ZrO2. *Physical Review Letters*, **2012**, 108, 116403 | 7.4 | 43 |
| 562 | Ab initio theory of phase stability and structural selectivity in Fe-Pd alloys. *Physical Review B*, **2012**, 85, | 3.3 | 31 |
| 561 | Prediction of A2BX4 metal-chalcogenide compounds via first-principles thermodynamics. *Physical Review B*, **2012**, 86, | 3.3 | 38 |
| 560 | 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 |
| 559 | Band or Polaron: The Hole Conduction Mechanism in the p-Type Spinel Rh2ZnO4. *Journal of the American Ceramic Society*, **2012**, 95, 269-274 | 3.8 | 43 |
| 558 | Influence of the atomic-scale structure on the exciton fine-structure splitting in InGaAs and GaAs quantum dots in a vertical electric field. *Physical Review B*, **2012**, 86, | 3.3 | 15 |
| 557 | Dissecting biexciton wave functions of self-assembled quantum dots by double-quantum-coherence optical spectroscopy. *Physical Review B*, **2012**, 86, | 3.3 | 9 |
| 556 | Genetic-algorithm discovery of a direct-gap and optically allowed superstructure from indirect-gap Si and Ge semiconductors. *Physical Review Letters*, **2012**, 108, 027401 | 7.4 | 86 |
| 555 | Comment on "Intrinsic n-type behavior in transparent conducting oxides: a comparative hybrid-functional study of In2O3, SnO2, and ZnO". *Physical Review Letters*, **2011**, 106, 069601; author reply 069602 | 7.4 | 32 |
| 554 | Localized interface states in coherent isovalent semiconductor heterojunctions. *Physical Review B*, **2011**, 84, | 3.3 | 11 |
| 553 | False-positive and false-negative assignments of topological insulators in density functional theory and hybrids. *Physical Review B*, **2011**, 84, | 3.3 | 86 |
| 552 | Matrix-embedded silicon quantum dots for photovoltaic applications: a theoretical study of critical factors. *Energy and Environmental Science*, **2011**, 4, 2546 | 35.4 | 65 |
| 551 | Learning to Predict Physical Properties using Sums of Separable Functions. *SIAM Journal of Scientific Computing*, **2011**, 33, 3381-3401 | 2.6 | 9 |
| 550 | Universal electrostatic origin of cation ordering in A2BO4 spinel oxides. *Journal of the American Chemical Society*, **2011**, 133, 11649-54 | 16.4 | 55 |
| 549 | Doping Rules and Doping Prototypes in A2BO4 Spinel Oxides. *Advanced Functional Materials*, **2011**, 21, 4493-4501 | 15.6 | 151 |
| 548 | Iron Chalcogenide Photovoltaic Absorbers. *Advanced Energy Materials*, **2011**, 1, 748-753 | 21.8 | 128 |
| 547 | Using design principles to systematically plan the synthesis of hole-conducting transparent oxides: Cu3VO4 and Ag3VO4 as a case study. *Physical Review B*, **2011**, 84, | 3.3 | 34 |
| 546 | Asymmetric cation nonstoichiometry in spinels: Site occupancy in Co2ZnO4 and Rh2ZnO4. *Physical Review B*, **2011**, 84, | 3.3 | 24 |

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| 545 | Geometry of epitaxial GaAs/(Al,Ga)As quantum dots as seen by excitonic spectroscopy. *Physical Review B*, **2011**, 84, | 3.3 | 13 |
| 544 | Absence of intrinsic spin splitting in one-dimensional quantum wires of tetrahedral semiconductors. *Physical Review B*, **2011**, 84, | 3.3 | 15 |
| 543 | Excitons and excitonic fine structures in Si nanowires: Prediction of an electronic state crossover with diameter changes. *Physical Review B*, **2011**, 84, | 3.3 | 10 |
| 542 | Altered reactivity and the emergence of ionic metal ordered structures in Li-Cs at high pressures. *Physical Review Letters*, **2010**, 104, 245501 | 7.4 | 13 |
| 541 | Bridging the gap between atomic microstructure and electronic properties of alloys: The case of (In,Ga)N. *Physical Review B*, **2010**, 82, | 3.3 | 35 |
| 540 | The electronic consequences of multivalent elements in inorganic solar absorbers: Multivalency of Sn in Cu2ZnSnS4. *Applied Physics Letters*, **2010**, 96, 201902 | 3.4 | 92 |
| 539 | Design principles and coupling mechanisms in the 2D quantum well topological insulator HgTe/CdTe. *Physical Review Letters*, **2010**, 105, 176805 | 7.4 | 22 |
| 538 | Discovery of a novel linear-in-k spin splitting for holes in the 2D GaAs/AlAs system. *Physical Review Letters*, **2010**, 104, 066405 | 7.4 | 30 |
| 537 | Many-body GW calculation of the oxygen vacancy in ZnO. *Physical Review B*, **2010**, 81, | 3.3 | 138 |
| 536 | Structure prediction and targeted synthesis: a new Na(n)N2 diazenide crystalline structure. *Journal of Chemical Physics*, **2010**, 133, 194504 | 3.9 | 16 |
| 535 | Dual nature of acceptors in GaN and ZnO: The curious case of the shallow MgGa deep state. *Applied Physics Letters*, **2010**, 96, 142114 | 3.4 | 88 |
| 534 | Wide InP nanowires with wurtzite/zincblende superlattice segments are type-II whereas narrower nanowires become type-I: an atomistic pseudopotential calculation. *Nano Letters*, **2010**, 10, 4055-60 | 11.5 | 68 |
| 533 | Long-Range Spin Currents with Chiral Crystals. *Physics Magazine*, **2010**, 3, | 1.1 | 180 |
| 532 | Generalized Koopmans density functional calculations reveal the deep acceptor state of NO in ZnO. *Physical Review B*, **2010**, 81, | 3.3 | 125 |
| 531 | Simple point-ion electrostatic model explains the cation distribution in spinel oxides. *Physical Review Letters*, **2010**, 105, 075501 | 7.4 | 40 |
| 530 | Effective band structure of random alloys. *Physical Review Letters*, **2010**, 104, 236403 | 7.4 | 144 |
| 529 | Nonstoichiometry and hole doping in NiO **2010**, | | 19 |
| 528 | Diagrammatic Separation of Different Crystal Structures of A2BX4 Compounds Without Energy Minimization: A Pseudopotential Orbital Radii Approach. *Advanced Functional Materials*, **2010**, 20, 1944-1952 | 15.6 | 41 |

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| 527 | Prediction of ordering and spontaneous rotation of epitaxial habits in substrate-coherent InGaN and GaAsSb. *Applied Physics Letters*, **2009**, 95, 081901 | 3.4 | 3 |
| 526 | Long-range order instead of phase separation in large lattice-mismatch isovalent AXBX systems. *Physical Review B*, **2009**, 80, | 3.3 | 5 |
| 525 | First-principles determination of low-temperature order and ground states of Fe-Ni, Fe-Pd, and Fe-Pt. *Physical Review B*, **2009**, 80, | 3.3 | 46 |
| 524 | Coexistence and coupling of zero-dimensional, two-dimensional, and continuum resonances in nanostructures. *Physical Review B*, **2009**, 80, | 3.3 | 20 |
| 523 | Electronic structure, donor and acceptor transitions, and magnetism of 3d impurities in In2O3 and ZnO. *Physical Review B*, **2009**, 79, | 3.3 | 93 |
| 522 | Rules of peak multiplicity and peak alignment in multiexcitonic spectra of (In,Ga)As quantum dots. *Physical Review B*, **2009**, 79, | 3.3 | 6 |
| 521 | II-VI oxides phase separate whereas the corresponding carbonates order: The stabilizing role of anionic groups. *Physical Review B*, **2009**, 80, | 3.3 | 3 |
| 520 | Spectral barcoding of quantum dots: Deciphering structural motifs from the excitonic spectra. *Physical Review B*, **2009**, 80, | 3.3 | 16 |
| 519 | Strain-induced localized states within the matrix continuum of self-assembled quantum dots. *Applied Physics Letters*, **2009**, 95, 023108 | 3.4 | 19 |
| 518 | Long- and short-range electron–hole exchange interaction in different types of quantum dots. *New Journal of Physics*, **2009**, 11, 123024 | 2.9 | 12 |
| 517 | Local density formalism approach to cohesive properties of solids: Diamond, BN, and LiF. *International Journal of Quantum Chemistry*, **2009**, 12, 539-546 | 2.1 | |
| 516 | Ternary semiconductors and ordered pseudobinary alloys: Electronic structure and predictions of new materials. *International Journal of Quantum Chemistry*, **2009**, 28, 629-653 | 2.1 | 5 |
| 515 | Atomistic pseudopotential calculations of thickness-fluctuation GaAs quantum dots. *Physical Review B*, **2009**, 79, | 3.3 | 19 |
| 514 | Direct observation of the structure of band-edge biexcitons in colloidal semiconductor CdSe quantum dots. *Physical Review B*, **2009**, 80, | 3.3 | 81 |
| 513 | Thermodynamic theory of epitaxial alloys: first-principles mixed-basis cluster expansion of (In, Ga)N alloy film. *Journal of Physics Condensed Matter*, **2009**, 21, 295402 | 1.8 | 11 |
| 512 | Polaronic hole localization and multiple hole binding of acceptors in oxide wide-gap semiconductors. *Physical Review B*, **2009**, 80, | 3.3 | 309 |
| 511 | Full-zone spin splitting for electrons and holes in bulk GaAs and GaSb. *Physical Review Letters*, **2009**, 102, 056405 | 7.4 | 35 |
| 510 | Predicting stable stoichiometries of compounds via evolutionary global space-group optimization. *Physical Review B*, **2009**, 80, | 3.3 | 45 |

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| 509 | Possible pitfalls in theoretical determination of ground-state crystal structures: The case of platinum nitride. *Physical Review B*, **2009**, 79, | 3.3 | 34 |
| 508 | Effect of atomic-scale randomness on the optical polarization of semiconductor quantum dots. *Physical Review B*, **2009**, 79, | 3.3 | 45 |
| 507 | Electronic correlation in anion p orbitals impedes ferromagnetism due to cation vacancies in Zn chalcogenides. *Physical Review Letters*, **2009**, 103, 016404 | 7.4 | 100 |
| 506 | Direct-bandgap InAs quantum-dots have long-range electron-hole exchange whereas indirect gap Si dots have short-range exchange. *Nano Letters*, **2009**, 9, 2648-53 | 11.5 | 11 |
| 505 | Accurate prediction of defect properties in density functional supercell calculations. *Modelling and Simulation in Materials Science and Engineering*, **2009**, 17, 084002 | 2 | 263 |
| 504 | Internal electronic structure and fine structure of multiexcitons in semiconductor quantum dots. *Physical Review B*, **2009**, 80, | 3.3 | 22 |
| 503 | Charge self-regulation upon changing the oxidation state of transition metals in insulators. *Nature*, **2008**, 453, 763-6 | 50.4 | 199 |
| 502 | Thermodynamic states and phase diagrams for bulk-incoherent, bulk-coherent, and epitaxially-coherent semiconductor alloys: Application to cubic (Ga,In)N. *Physical Review B*, **2008**, 77, | 3.3 | 60 |
| 501 | Theoretical and experimental examination of the intermediate-band concept for strain-balanced (In,Ga)As/Ga(As,P) quantum dot solar cells. *Physical Review B*, **2008**, 78, | 3.3 | 182 |
| 500 | Intrinsic DX centers in ternary chalcopyrite semiconductors. *Physical Review Letters*, **2008**, 100, 016401 | 7.4 | 120 |
| 499 | Relative stability, electronic structure, and magnetism of MnN and (Ga,Mn)N alloys. *Physical Review B*, **2008**, 78, | 3.3 | 34 |
| 498 | Control of ferromagnetism via electron doping in In2O3:Cr. *Physical Review Letters*, **2008**, 101, 027203 | 7.4 | 61 |
| 497 | Highly reduced fine-structure splitting in InAs/InP quantum dots offering an efficient on-demand entangled 1.55-microm photon emitter. *Physical Review Letters*, **2008**, 101, 157405 | 7.4 | 53 |
| 496 | 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 |
| 495 | 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 |
| 494 | Carrier multiplication in semiconductor nanocrystals: theoretical screening of candidate materials based on band-structure effects. *Nano Letters*, **2008**, 8, 3174-81 | 11.5 | 68 |
| 493 | 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 |
| 492 | Examining F□ster Energy Transfer for Semiconductor Nanocrystalline Quantum Dot Donors and Acceptors. *Journal of Physical Chemistry C*, **2008**, 112, 13336-13341 | 3.8 | 97 |

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| 491 | Pseudopotential calculations of band gaps and band edges of short-period (InAs)n(GaSb)m superlattices with different substrates, layer orientations, and interfacial bonds. *Physical Review B*, **2008**, 77, | 3.3 | 31 |
| 490 | Quantum-size-induced electronic transitions in quantum dots: Indirect band-gap GaAs. *Physical Review B*, **2008**, 78, | 3.3 | 27 |
| 489 | Finding the lowest-energy crystal structure starting from randomly selected lattice vectors and atomic positions: first-principles evolutionary study of the AuPd, CdPt, AlSc, CuPd, PdTi, and IrN binary systems. *Journal of Physics Condensed Matter*, **2008**, 20, 295212 | 1.8 | 25 |
| 488 | Excited-state relaxation in PbSe quantum dots. *Journal of Chemical Physics*, **2008**, 128, 164720 | 3.9 | 43 |
| 487 | Limitation of the open-circuit voltage due to metastable intrinsic defects in Cu(In,Ga)Se2 and strategies to avoid these defects. *Conference Record of the IEEE Photovoltaic Specialists Conference*, **2008**, | | 3 |
| 486 | Using superlattice ordering to reduce the band gap of random (In,Ga)As/InP alloys to a target value via the inverse band structure approach. *Physical Review B*, **2008**, 78, | 3.3 | 4 |
| 485 | Identifying the minimum-energy atomic configuration on a lattice: Lamarckian twist on Darwinian evolution. *Physical Review B*, **2008**, 78, | 3.3 | 32 |
| 484 | Band-gap design of quaternary (In,Ga)(As,Sb) semiconductors via the inverse-band-structure approach. *Physical Review Letters*, **2008**, 100, 186403 | 7.4 | 40 |
| 483 | Origins of the doping asymmetry in oxides: Hole doping in NiO versus electron doping in ZnO. *Physical Review B*, **2007**, 75, | 3.3 | 182 |
| 482 | Lifetime and polarization of the radiative decay of excitons, biexcitons, and trions in CdSe nanocrystal quantum dots. *Physical Review B*, **2007**, 75, | 3.3 | 87 |
| 481 | Origins of the p-type nature and cation deficiency in Cu2O and related materials. *Physical Review B*, **2007**, 76, | 3.3 | 402 |
| 480 | New insights on chalcopyrites from solid-state theory. *Thin Solid Films*, **2007**, 515, 6160-6162 | 2.2 | 20 |
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