Alexander Zunger

List of Publications by Year
in descending order

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666	84,881	518	559
papers	citations	131 h-index	270 g-index

677	677	677	46447
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Intrinsic doping limitations in inorganic lead halide perovskites. Materials Horizons, 2022, 9, 791-803.	6.4	10
2	Bulk <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>NdNi</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> is thermodynamically unstable with respect to decomposition while hydrogenation reduces the	1.1	33
3	Intrinsic local symmetry breaking in nominally cubic paraelectric <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>EuTi</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review Materials, 2022, 6, .	0.9	8
4	Dependence of band gaps in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>d</mml:mi></mml:math> -electron perovskite oxides on magnetism. Physical Review B, 2022, 105, .	1.1	6
5	Intrinsic local symmetry breaking in nominally cubic paraelectric <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>BaTi</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2022, 105, .	1.1	10
6	Prediction of low-Z collinear and noncollinear antiferromagnetic compounds having momentum-dependent spin splitting even without spin-orbit coupling. Physical Review Materials, 2021, 5, .	0.9	64
7	Understanding Doping of Quantum Materials. Chemical Reviews, 2021, 121, 3031-3060.	23.0	86
8	Mass enhancement in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:r and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>s</mml:mi><mml:mtext>â^'</mml:mtext><mml:mi>p</mml:m perovskites from symmetry breaking. Physical Review B, 2021, 103, .	1.1	24
9	Strong influence of nonmagnetic ligands on the momentum-dependent spin splitting in antiferromagnets. Physical Review B, 2021, 103, .	1.1	16
10	Effect of static local distortions vs. dynamic motions on the stability and band gaps of cubic oxide and halide perovskites. Materials Today, 2021, 49, 107-122.	8.3	37
11	Different shapes of spin textures as a journey through the Brillouin zone. Physical Review B, 2021, 104, .	1.1	23
12	Piezoelectricity in nominally centrosymmetric phases. Physical Review Research, 2021, 3, .	1.3	19
13	Realization of predicted exotic materials: The burden of proof. Materials Today, 2020, 32, 35-45.	8.3	29
14	The Rashba Scale: Emergence of Band Anti-crossing as a Design Principle for Materials with Large Rashba Coefficient. Matter, 2020, 3, 145-165.	5.0	21
15	Symmetry-breaking polymorphous descriptions for correlated materials without interelectronic U. Physical Review B, 2020, 102, .	1.1	48
16	Giant momentum-dependent spin splitting in centrosymmetric low- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Z</mml:mi></mml:math> antiferromagnets. Physical Review B, 2020, 102, .	1.1	101
17	Inverse design of compounds that have simultaneously ferroelectric and Rashba cofunctionality. Physical Review B, 2020, 102, .	1.1	20
18	False metals, real insulators, and degenerate gapped metals. Applied Physics Reviews, 2020, 7, .	5.5	44

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19	Understanding electronic peculiarities in tetragonal FeSe as local structural symmetry breaking. Physical Review B, 2020, 102, .	1.1	26
20	Hole antidoping of oxides. Physical Review B, 2020, 101, .	1.1	10
21	Polymorphous nature of cubic halide perovskites. Physical Review B, 2020, 101, .	1.1	104
22	Ferri-chiral compounds with potentially switchable Dresselhaus spin splitting. Physical Review B, 2020, 102, .	1.1	4
23	Digging for topological property in disordered alloys: the emergence of Weyl semimetal phase and sequential band inversions in PbSeâ€“SnSe alloys. Materials Horizons, 2019, 6, 2124-2134.	6.4	15
24	Mott gapping in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi><mml:mspace width="0.16em" /><mml:mi>A</mml:mi><mml:mi>B</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> perovskites without Mott-Hubbard interelectronic repulsion energy U. Physical Review B, 2019, 100, .	1.1	70
25	Spontaneous Non-stoichiometry and Ordering in Degenerate but Gapped Transparent Conductors. Matter, 2019, 1, 280-294.	5.0	27
26	Beware of plausible predictions of fantasy materials. Nature, 2019, 566, 447-449.	13.7	64
27	Design of Mixedâ€Cation Triâ€Layered Pbâ€Free Halide Perovskites for Optoelectronic Applications. Advanced Electronic Materials, 2019, 5, 1900234.	2.6	21
28	Antidoping in Insulators and Semiconductors Having Intermediate Bands with Trapped Carriers. Physical Review Letters, 2019, 122, 106403.	2.9	28
29	Origin of band gaps in 3d perovskite oxides. Nature Communications, 2019, 10, 1658.	5.8	154
30	Uncovering and tailoring hidden Rashba spinâ€“orbit splitting in centrosymmetric crystals. Nature Communications, 2019, 10, 906.	5.8	53
31	Formation and Composition-Dependent Properties of Alloys of Cubic Halide Perovskites. Chemistry of Materials, 2019, 31, 2497-2506.	3.2	48
32	Alloy theory with atomic resolution for Rashba or topological systems. Physical Review Materials, 2019, 3, .	0.9	3
33	Origins versus fingerprints of the Jahn-Teller effect in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>d</mml:mi></mml:math> -electron <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>A</mml:mi><mml:mi>B</mml:mi><mml:msub><mml:mi> perovskites. Physical Review Research, 2019, 1, .	1.3	31
34	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, .	1.1	100
35	Inverse design in search of materials with target functionalities. Nature Reviews Chemistry, 2018, 2, .	13.8	235
36	Topological Insulators versus Topological Dirac Semimetals in Honeycomb Compounds. Journal of the American Chemical Society, 2018, 140, 13687-13694.	6.6	42

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37	Electron Doping of Proposed Kagome Quantum Spin Liquid Produces Localized States in the Band Gap. Physical Review Letters, 2018, 121, 186402.	2.9	21
38	Bond disproportionation, charge self-regulation, and ligand holes in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>s</mml:mi><mml:mtext>â^'</mml:mtext><mml:mi>p</mml:mi></mml:mrow></mml:math> and in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>d</mml:mi></mml:math> -electron <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>A</mml:mi><mml:mi>B</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> perovskite compounds by combining machine learning and density functional theory. Physical Review Materials, 2018, 2, .	1.1	45
39	Discovery of new <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>A</mml:mi><mml:mi>B</mml:mi><mml:mi mathvariant="italic">AB</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> perovskite compounds by combining machine learning and density functional theory. Physical Review Materials, 2018, 2, .	0.9	127
40	Natural off-stoichiometry causes carrier doping in half-Heusler filled tetrahedral structures. Physical Review B, 2017, 95, .	1.1	61
41	Cuâ€“In Halide Perovskite Solar Absorbers. Journal of the American Chemical Society, 2017, 139, 6718-6725.	6.6	316
42	Functionality-Directed Screening of Pb-Free Hybrid Organicâ€“Inorganic Perovskites with Desired Intrinsic Photovoltaic Functionalities. Chemistry of Materials, 2017, 29, 524-538.	3.2	135
43	CuTaS₃: Intermetal dâ€“d Transitions Enable High Solar Absorption. Chemistry of Materials, 2017, 29, 2594-2598.	3.2	21
44	Absence of redshift in the direct bandgap of silicon nanocrystals with reduced size. Nature Nanotechnology, 2017, 12, 930-932.	15.6	22
45	Predicted electronic markers for polytypes of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>LaOBi</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> examined via angle-resolved photoemission spectroscopy. Physical Review B, 2017, 95, .	1.1	18
46	Rapid Transition of the Hole Rashba Effect from Strong Field Dependence to Saturation in Semiconductor Nanowires. Physical Review Letters, 2017, 119, 126401.	2.9	21
47	The Enabling Electronic Motif for Topological Insulation in ABO 3 Perovskites. Advanced Functional Materials, 2017, 27, 1701266.	7.8	21
48	Predicted Realization of Cubic Dirac Fermion in Quasi-One-Dimensional Transition-Metal Monochalcogenides. Physical Review X, 2017, 7, .	2.8	72
49	Instilling defect tolerance in new compounds. Nature Materials, 2017, 16, 964-967.	13.3	219
50	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, .	0.9	43
51	Transforming Common IIIâ€“V and IIâ€“VI Semiconductor Compounds into Topological Heterostructures: The Case of CdTe/InSb Superlattices. Advanced Functional Materials, 2016, 26, 3259-3267.	7.8	27
52	Orbital mapping of energy bands and the truncated spin polarization in three-dimensional Rashba semiconductors. Physical Review B, 2016, 94, .	1.1	11
53	Minimal ingredients for orbital-texture switches at Dirac points in strong spinâ€“orbit coupled materials. Npj Quantum Materials, 2016, 1, .	1.8	7
54	Polytypism inLaOBiS2-type compounds based on different three-dimensional stacking sequences of two-dimensionalBiS2layers. Physical Review B, 2016, 93, .	1.1	34

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55	Single-dot absorption spectroscopy and theory of silicon nanocrystals. Physical Review B, 2016, 93, .	1.1	39
56	Strong Absorption Enhancement in Si Nanorods. Nano Letters, 2016, 16, 7937-7941.	4.5	11
57	Quasi-Direct Optical Transitions in Silicon Nanocrystals with Intensity Exceeding the Bulk. Nano Letters, 2016, 16, 1583-1589.	4.5	62
58	Search and design of nonmagnetic centrosymmetric layered crystals with large local spin polarization. Physical Review B, 2015, 91, .	1.1	51
59	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, .	1.1	10
60	Supercoupling between heavy-hole and light-hole states in nanostructures. Physical Review B, 2015, 92, .	1.1	31
61	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, .	1.1	4
62	Intrinsic Transparent Conductors without Doping. Physical Review Letters, 2015, 115, 176602.	2.9	36
63	Cation ordering induced polarization enhancement for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>PbTiO</mml:mi><mml:mn>3</mml:mn></mml:msub><m superlattices. Physical Review B, 2015, 91, .	1.1	6
64	Switching a Normal Insulator into a Topological Insulator via Electric Field with Application to Phosphorene. Nano Letters, 2015, 15, 1222-1228.	4.5	406
65	Evolution of Electronic Structure as a Function of Layer Thickness in Group-VIB Transition Metal Dichalcogenides: Emergence of Localization Prototypes. Nano Letters, 2015, 15, 949-957.	4.5	72
66	Intrinsic Circular Polarization in Centrosymmetric Stacks of Transition-Metal Dichalcogenide Compounds. Physical Review Letters, 2015, 114, 087402.	2.9	53
67	Split Dirac cones in HgTe/CdTe quantum wells due to symmetry-enforced level anticrossing at interfaces. Physical Review B, 2015, 91, .	1.1	67
68	Design and discovery of a novel half-Heusler transparent hole conductor made of all-metallic heavy elements. Nature Communications, 2015, 6, 7308.	5.8	89
69	Prediction and accelerated laboratory discovery of previously unknown 18-electron ABX compounds. Nature Chemistry, 2015, 7, 308-316.	6.6	349
70	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, 11383-11390.	6.6	12
71	Research Update: Towards designed functionalities in oxide-based electronic materials. APL Materials, 2015, 3, .	2.2	26
72	Reinterpretation of the Expected Electronic Density of States of Semiconductor Nanowires. Nano Letters, 2015, 15, 88-95.	4.5	9

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73	Hidden spin polarization in inversion-symmetric bulk crystals. Nature Physics, 2014, 10, 387-393.	6.5	400
74	Assessing capability of semiconductors to split water using ionization potentials and electron affinities only. Physical Chemistry Chemical Physics, 2014, 16, 3706.	1.3	226
75	Structurally unstable<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mi>A</mml:mi><mml:mi>III</mml:mi></mml:msup><mml:ms mathvariant="normal">BiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>perovskites are predicted to be topological insulators but their stable structural forms are trivial band insulators. Physical Review B, 2014, 90, .	1.1	21
76	A polarity-induced defect mechanism for conductivity and magnetism at polarâ€“nonpolar oxide interfaces. Nature Communications, 2014, 5, 5118.	5.8	247
77	Self-Doping and Electrical Conductivity in Spinel Oxides: Experimental Validation of Doping Rules. Chemistry of Materials, 2014, 26, 1867-1873.	3.2	35
78	2D optical photon echo spectroscopy of a selfâ€assembled quantum dot. Annalen Der Physik, 2013, 525, 31-42.	0.9	11
79	Crystal structures and metastability of carbon-boron compounds C<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>B and C<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>5</mml:mn></mml:msub></mml:math>B. Physical Review B, 2013, 87, .	1.1	22
80	Liâ€Doped Cr₂MnO₄: A New pâ€Type Transparent Conducting Oxide by Computational Materials Design. Advanced Functional Materials, 2013, 23, 5267-5276.	7.8	57
81	Theoretical Prediction and Experimental Realization of New Stable Inorganic Materials Using the Inverse Design Approach. Journal of the American Chemical Society, 2013, 135, 10048-10054.	6.6	111
82	Inverse Design of High Absorption Thinâ€Film Photovoltaic Materials. Advanced Energy Materials, 2013, 3, 43-48.	10.2	316
83	Genetic design of enhanced valley splitting towards a spin qubit in silicon. Nature Communications, 2013, 4, 2396.	5.8	49
84	On the Nature of the Magnetism-Promoting States in Dilute Magnetic Semiconductor and Oxide Thin Films. Journal of Nanoelectronics and Optoelectronics, 2013, 8, 466-471.	0.1	1
85	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, .	1.1	17
86	Dissecting biexciton wave functions of self-assembled quantum dots by double-quantum-coherence optical spectroscopy. Physical Review B, 2012, 86, .	1.1	10
87	Genetic-Algorithm Discovery of a Direct-Gap and Optically Allowed Superstructure from Indirect-Gap Si and Ge Semiconductors. Physical Review Letters, 2012, 108, 027401.	2.9	103
88	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.	1.1	9
89	Extracting<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>E</mml:mi></mml:math>versus<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mover accent="true"><mml:mi>k</mml:mi><mml:mo>âƒ—</mml:mo></mml:mover></mml:math>effective band structure from supercell calculations on alloys and impurities. Physical Review B, 2012, 85, .	1.1	338
90	Correcting density functional theory for accurate predictions of compound enthalpies of formation: Fitted elemental-phase reference energies. Physical Review B, 2012, 85, .	1.1	454

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91	Genomic Design of Strong Direct-Gap Optical Transition in Si/Ge Core/Multishell Nanowires. Nano Letters, 2012, 12, 984-991.	4.5	54
92	Band-structure, optical properties, and defect physics of the photovoltaic semiconductor SnS. Applied Physics Letters, 2012, 100, .	1.5	382
93	Identification of Potential Photovoltaic Absorbers Based on First-Principles Spectroscopic Screening of Materials. Physical Review Letters, 2012, 108, 068701.	2.9	497
94	Angle-resolved photoemission and quasiparticle calculation of ZnO: The need for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>d</mml:mi></mml:math>band shift in oxide semiconductors. Physical Review B, 2012, 86, .	1.1	56
95	Large insulating gap in topological insulators induced by negative spin-orbit splitting. Physical Review B, 2012, 86, .	1.1	26
96	Two-Dimensional Polaronic Behavior in the Binary Oxides<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>m</mml:mi><mml:mtext mathvariant="normal">â^’</mml:mtext><mml:msub><mml:mi>HfO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>m</mml:mi><mml:mtext mathvariant="normal">â^’</mml:mtext><mml:msub><mml:mi>ZrO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2012, 108, 116403.	2.9	56
97	Ab initiotheory of phase stability and structural selectivity in Fe-Pd alloys. Physical Review B, 2012, 85, .	1.1	36
98	Prediction of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>A</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi>B</mml:mi></mml:mrow></mml:msub> compounds via first-principles thermodynamics. Physical Review B, 2012, 86, .	1.1	46
99	Sorting Stable versus Unstable Hypothetical Compounds: The Case of Multiâ€Functional ABX Halfâ€Heusler Filled Tetrahedral Structures. Advanced Functional Materials, 2012, 22, 1425-1435.	7.8	107
100	Band or Polaron: The Hole Conduction Mechanism in the pâ€Type Spinel <scp><scp>Rh₂ZnO₄</scp></scp>. Journal of the American Ceramic Society, 2012, 95, 269-274.	1.9	48
101	Co3O4â€“Co2ZnO4 spinels: The case for a solid solution. Journal of Solid State Chemistry, 2012, 190, 143-149.	1.4	15
102	Using design principles to systematically plan the synthesis of hole-conducting transparent oxides: Cu<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>VO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>and Ag<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>PO4	1.1	38
103	Comment on "Origin of Intrinsic n-Type Behavior in Transparent Conducting Oxides: A Comparative Hybrid-Functional Study ofIn2O3,SnO2, and ZnOâ€. Physical Review Letters, 2011, 106, 069601; author reply 069602.	2.9	33
104	Localized interface states in coherent isovalent semiconductor heterojunctions. Physical Review B, 2011, 84, .	1.1	11
105	False-positive and false-negative assignments of topological insulators in density functional theory and hybrids. Physical Review B, 2011, 84, .	1.1	93
106	Matrix-embedded silicon quantum dots for photovoltaic applications: a theoretical study of critical factors. Energy and Environmental Science, 2011, 4, 2546.	15.6	72
107	Learning to Predict Physical Properties using Sums of Separable Functions. SIAM Journal of Scientific Computing, 2011, 33, 3381-3401.	1.3	10
108	Universal Electrostatic Origin of Cation Ordering in A₂BO₄ Spinel Oxides. Journal of the American Chemical Society, 2011, 133, 11649-11654.	6.6	71

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109	Doping Rules and Doping Prototypes in A₂BO₄ Spinel Oxides. Advanced Functional Materials, 2011, 21, 4493-4501.	7.8	176
110	Iron Chalcogenide Photovoltaic Absorbers. Advanced Energy Materials, 2011, 1, 748-753.	10.2	138
111	Publisherâ€™s Note: Localized interface states in coherent isovalent semiconductor heterojunctions [Phys. Rev. B84, 125315 (2011)]. Physical Review B, 2011, 84, .	1.1	0
112	Asymmetric cation nonstoichiometry in spinels: Site occupancy in Co<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>ZnO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>and Rh<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:	1.1	25
113	Geometry of epitaxial GaAs/(Al,Ga)As quantum dots as seen by excitonic spectroscopy. Physical Review B, 2011, 84, .	1.1	16
114	Absence of intrinsic spin splitting in one-dimensional quantum wires of tetrahedral semiconductors. Physical Review B, 2011, 84, .	1.1	24
115	Excitons and excitonic fine structures in Si nanowires: Prediction of an electronic state crossover with diameter changes. Physical Review B, 2011, 84, .	1.1	15
116	Nonstoichiometry and hole doping in NiO. AIP Conference Proceedings, 2010, , .	0.3	24
117	Diagrammatic Separation of Different Crystal Structures of A₂BX₄ Compounds Without Energy Minimization: A Pseudopotential Orbital Radii Approach. Advanced Functional Materials, 2010, 20, 1944-1952.	7.8	51
118	Altered Reactivity and the Emergence of Ionic Metal Ordered Structures in Li-Cs at High Pressures. Physical Review Letters, 2010, 104, 245501.	2.9	17
119	Bridging the gap between atomic microstructure and electronic properties of alloys: The case of (In,Ga)N. Physical Review B, 2010, 82, .	1.1	39
120	The electronic consequences of multivalent elements in inorganic solar absorbers: Multivalency of Sn in Cu2ZnSnS4. Applied Physics Letters, 2010, 96, .	1.5	113
121	Design Principles and Coupling Mechanisms in the 2D Quantum Well Topological InsulatorHgTe/CdTe. Physical Review Letters, 2010, 105, 176805.	2.9	31
122	Discovery of a Novel Linear-in-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>k</mml:mi></mml:math>Spin Splitting for Holes in the 2D<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>GaAs</mml:mi><mml:mo>/</mml:mo><mml:mi>AlAs</mml:mi></mml:math>System. Physical Review Letters, 2010, 104, 066405.	2.9	41
123	Many-body<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>calculation of the oxygen vacancy in ZnO. Physical Review B, 2010, 81, .	1.1	147
124	Structure prediction and targeted synthesis: A new NanN2 diazenide crystalline structure. Journal of Chemical Physics, 2010, 133, 194504.	1.2	17
125	Dual nature of acceptors in GaN and ZnO: The curious case of the shallow MgGa deep state. Applied Physics Letters, 2010, 96, .	1.5	101
126	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, 4055-4060.	4.5	76

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127	Generalized Koopmans density functional calculations reveal the deep acceptor state of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>N</mml:mtext><mml:mtext>O</mml:mtext></mml:msub></mml:mrow></m ZnO. Physical Review B, 2010, 81, .	1.1	135
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