Mao-Hua Du

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1818974/publications.pdf

Version: 2024-02-01

		29994	34900
169	10,636	54	98
papers	citations	h-index	g-index

176	176	176	11702
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Tuning the room temperature ferromagnetism in Fe₅GeTe₂ by arsenic substitution. 2D Materials, 2022, 9, 015013.	2.0	14
2	(C₇H₁₁N₂)₂MBr₄ (M=Cu, Zn): Xâ€Ray Sensitive 0D Hybrid Metal Halides with Tunable Broadband Emission. European Journal of Inorganic Chemistry, 2022, 2022, e202100954.	1.0	11
3	Crystal growth, density functional theory, and scintillation properties of TlMgX3 (XÂ=ÂCl, Br, I). Chemical Physics, 2022, 558, 111535.	0.9	2
4	Surfaceâ€Driven Evolution of the Anomalous Hall Effect in Magnetic Topological Insulator MnBi₂Te₄ Thin Films. Advanced Functional Materials, 2022, 32, .	7.8	2
5	Tuning Fermi Levels in Intrinsic Antiferromagnetic Topological Insulators MnBi₂Te₄ and MnBi₄Te₇ by Defect Engineering and Chemical Doping. Advanced Functional Materials, 2021, 31, 2006516.	7.8	68
6	TlSr2I5:Eu2+- A new high density scintillator for gamma-ray detection. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2021, 988, 164876.	0.7	7
7	Crystal growth and scintillation properties of pure and Tl-doped Cs3Cu2I5. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2021, 991, 164963.	0.7	35
8	Zero-Dimensional Hybrid Organicâ€“Inorganic Indium Bromide with Blue Emission. Inorganic Chemistry, 2021, 60, 1045-1054.	1.9	48
9	Crystal growth, density functional theory, and scintillation properties of Tl3LnCl6:Ce3+ and TlLn2Cl7:Ce3+ (Ln = Y, Gd). Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2021, 995, 165047.	0.7	11
10	Intrinsic and complex defect engineering of quasi-one-dimensional ribbons <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Sb</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>3</mml:mn></mml:mrow></mml:math> for photovoltaics performance. Physical Review Materials, 2021, 5, .	0.9	9
11	Hierarchical excitations from correlated spin tetrahedra on the breathing pyrochlore lattice. Physical Review B, 2021, 103, .	1.1	5
12	(NH₄)₂AgX₃ (X = Br, I): 1D Silver Halides with Broadband White Light Emission and Improved Stability. ACS Materials Au, 2021, 1, 62-68.	2.6	14
13	Magnetic properties of the Shastry-Sutherland lattice material <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>BaNd</mml:mi><mml:mn>2</mml:mn></ Physical Review Materials, 2021, 5, .	0.9	7
14	Design of High-Performance Lead-Free Quaternary Antiperovskites for Photovoltaics via Ion Type Inversion and Anion Ordering. Journal of the American Chemical Society, 2021, 143, 12369-12379.	6.6	24
15	Metal Halide Scaffolded Assemblies of Organic Molecules with Enhanced Emission and Room Temperature Phosphorescence. Journal of Physical Chemistry Letters, 2021, 12, 8229-8236.	2.1	27
16	Role of Polycyclic Aromatic Alkylammonium Cations in Tuning the Electronic Properties and Band Alignment of Two-Dimensional Hybrid Perovskite Semiconductors. Journal of Physical Chemistry Letters, 2021, 12, 9754-9760.	2.1	8
17	Compositionâ€Dependent Photoluminescence Properties and Antiâ€Counterfeiting Applications of A₂AgX₃ (AÂ=ÂRb, Cs; XÂ= ÂCl, Br, I). Advanced Functional Materials, 2021, 31, 2104941.	7.8	50
18	Photophysical properties of zero-dimensional perovskites studied by PBE0 and GW+BSE methods. Journal of Applied Physics, 2021, 130, 203106.	1.1	4

#	Article	IF	Citations
19	Rb₂CuX₃ (X = Cl, Br): 1D Allâ€•Inorganic Copper Halides with Ultrabright Blue Emission and Upâ€Conversion Photoluminescence. Advanced Optical Materials, 2020, 8, 1901338.	3.6	86
20	Emission Trend of Multiple Self-Trapped Excitons in Luminescent 1D Copper Halides. ACS Energy Letters, 2020, 5, 464-469.	8.8	111
21	Crystal Synthesis and Frustrated Magnetism in Triangular Lattice CsRESe₂ (RE = Laâ€“Lu): Quantum Spin Liquid Candidates CsCeSe₂ and CsYbSe₂. , 2020, 2, 71-75.		49
22	(INVITED) First-principles calculations of quantum transitions at local centers. Optical Materials: X, 2020, 8, 100066.	0.3	5
23	Reaching 90% Photoluminescence Quantum Yield in One-Dimensional Metal Halide C₄N₂H₁₄PbBr₄ by Pressure-Suppressed Nonradiative Loss. Journal of the American Chemical Society, 2020, 142, 16001-16006.	6.6	109
24	Flat bands in the CoSn-type compounds. Physical Review B, 2020, 102, .	1.1	52
25	Deciphering the effect of traps on electronic charge transport properties of methylammonium lead tribromide perovskite. Science Advances, 2020, 6, .	4.7	47
26	0D and 2D: The Cases of Phenylethylammonium Tin Bromide Hybrids. Chemistry of Materials, 2020, 32, 4692-4698.	3.2	72
27	Robust Ferromagnetism in Highly Strained <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>SrCoO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn> Thin Films. Physical Review X, 2020, 10, .	2.8	15
28	K₂CuX₃ (X = Cl, Br): All-Inorganic Lead-Free Blue Emitters with Near-Unity Photoluminescence Quantum Yield. Chemistry of Materials, 2020, 32, 6197-6205.	3.2	109
29	Role of Lithium Codoping in Enhancing the Scintillation Yield of Aluminate Garnets. Physical Review Applied, 2020, 13, .	1.5	8
30	Thallium-based scintillators for high-resolution gamma-ray spectroscopy: Ce<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e576" altimg="si37.svg"><mml:msup><mml:mrow /><mml:mrow><mml:mn>3</mml:mn><mml:mo>+</mml:mo></mml:mrow></mml:msup></mml:math>-doped Tl2LaCl5 and Tl2LaBr<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e596" altimg="si12.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>5</mml:mn>	0.7	9
31	Additive-assisted synthesis and optoelectronic properties of (CH3NH3)4Bi6I22. Inorganic Chemistry Frontiers, 2020, 7, 1564-1572.	3.0	11
32	Density functional studies of defects and defect-related luminescence in Mg3N2. Physical Review Materials, 2020, 4, .	0.9	2
33	Tuning magnetic order in the van der Waals metal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Fe</mml:mi><mml:mn>5</mml:mn> by cobalt substitution. Physical Review Materials, 2020, 4, .	3.9	52
34	Adsorption-controlled growth of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>MnTe</mml:mi><mml:msub><mml:mrow><mml:mo>(</m by molecular beam epitaxy exhibiting stoichiometry-controlled magnetism. Physical Review Materials, 2020, 4, .	0.9	15
35	Native defects in antiferromagnetic topological insulator <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>MnBi</mml:mi><mml:mn>2</mml:mn> Physical Review Materials, 2020, 4, .	3.9	40
36	Atomic-Scale Study of Intrinsic Defects Suppressing the Thermal Conductivity of Boron Arsenide. Microscopy and Microanalysis, 2019, 25, 942-943.	0.2	0

#	Article	IF	Citations
37	Highly Efficient Broad-Band Luminescence Involving Organic and Inorganic Molecules in a Zero-Dimensional Hybrid Lead Chloride. Journal of Physical Chemistry C, 2019, 123, 22470-22477.	1.5	57
38	Frontispiece: (CH₃NH₃)AuX₄â‹…H₂O (X=Cl, Br) and (CH₃NH₃)AuCl₄: Lowâ€Band Gap Leadâ€Free Layered Gold Halide Perovskite Materials. Chemistry - A European Journal, 2019, 25, .	1.7	0
39	Bulk Assembly of Zero-Dimensional Organic Lead Bromide Hybrid with Efficient Blue Emission. , 2019, 1, 594-598.		92
40	Bright Luminescence from Nontoxic CsCu₂X₃ (X = Cl, Br, I). , 2019, 1, 459-465.		148
41	Chemical Trend of Transition-Metal Doping in WSe2. Physical Review Applied, 2019, 12, .	1.5	16
42	Green Emitting Single-Crystalline Bulk Assembly of Metal Halide Clusters with Near-Unity Photoluminescence Quantum Efficiency. ACS Energy Letters, 2019, 4, 1579-1583.	8.8	117
43	(CH 3 NH 3)AuX 4 â‹…H 2 O (X=Cl, Br) and (CH 3 NH 3)AuCl 4 : Lowâ€Band Gap Leadâ€Free Layered Gold Halide Perovskite Materials. Chemistry - A European Journal, 2019, 25, 9875-9884.	1.7	15
44	Zero-dimensional metal oxide Li4TiO4. Journal of Materials Chemistry C, 2019, 7, 5710-5715.	2.7	11
45	Near-Unity Photoluminescence Quantum Yield in Blue-Emitting Cs₃Cu₂Br_{5â€“x}I_x (0 â‰¤ x â‰¤ 5). ACS Applied Electronic Materials, 2019, 1, 269-274.	2.0	184
46	Hybrid Organicâ€“Inorganic Halides (C₅H₇N₂)₂MBr₄ (M = Hg, Zn) with High Color Rendering Index and High-Efficiency White-Light Emission. Chemistry of Materials, 2019, 31, 2983-2991.	3.2	143
47	Rb₄Ag₂BiBr₉: A Lead-Free Visible Light Absorbing Halide Semiconductor with Improved Stability. Inorganic Chemistry, 2019, 58, 4446-4455.	1.9	35
48	Microscopic origin of multiple exciton emission in low-dimensional lead halide perovskites. Journal of Chemical Physics, 2019, 151, 181101.	1.2	23
49	Electronic shell structures, self-trapped excitons, and defect-bound excitons in Li₂B₁₂H₁₂. Journal of Materials Chemistry C, 2019, 7, 14342-14349.	2.7	8
50	Low dimensional metal halide perovskites and hybrids. Materials Science and Engineering Reports, 2019, 137, 38-65.	14.8	300
51	Excitation Energies of Localized Correlated Defects via Quantum Monte Carlo: A Case Study of Mn⁴⁺-Doped Phosphors. Journal of Physical Chemistry Letters, 2019, 10, 67-74.	2.1	15
52	Bulk Assembly of Corrugated 1D Metal Halides with Broadband Yellow Emission. Advanced Optical Materials, 2019, 7, 1801474.	3.6	65
53	Intense deep-red zero phonon line emission of Mn⁴⁺ in double perovskite La₄Ti₃O₁₂. Physical Chemistry Chemical Physics, 2019, 21, 25108-25117.	1.3	21
54	Impact of metal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">n</mml:mi><mml:msup><mml:mrow><mml:mi mathvariant="normal">s</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msup></mml:mrow></mml:math> lone pair on luminescence quantum efficiency in low-dimensional halide perovskites. Physical Review Materials, 2019, 3, .	0.9	60

#	Article	IF	Citations
55	Optoelectronic properties of candidate photovoltaic Cu2PbSiS4, Ag2PbGeS4 and KAg2SbS4 semiconductors. Journal of Alloys and Compounds, 2018, 746, 405-412.	2.8	10
56	Tuning the Magnetic Properties and Structural Stabilities of the 2-17-3 Magnets<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

#	Article	IF	Citations
73	Zero-dimensional Cs₄EuX₆ (X = Br, I) all-inorganic perovskite single crystals for gamma-ray spectroscopy. Journal of Materials Chemistry C, 2018, 6, 6647-6655.	2.7	66
74	Self-Activated Low-Dimensional Metal Halide Phosphors and Scintillators. ECS Meeting Abstracts, 2018, , .	0.0	0
75	Influence of defects and dopants on the photovoltaic performance of Bi₂S₃: first-principles insights. Journal of Materials Chemistry A, 2017, 5, 6200-6210.	5.2	97
76	Impurity-induced deep centers in Tl6SI4. Journal of Applied Physics, 2017, 121, 145102.	1.1	9
77	Synthesis, Crystal and Electronic Structures, and Optical Properties of (CH₃NH₃)₂CdX₄ (X = Cl, Br, I). Inorganic Chemistry, 2017, 56, 13878-13888.	1.9	78
78	Bulk assembly of organic metal halide nanotubes. Chemical Science, 2017, 8, 8400-8404.	3.7	76
79	Prospective high thermoelectric performance of the heavily <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="bold-italic">p</mml:mi></mml:math> -doped half-Heusler compound CoVSn. Physical Review B, 2017, 95, .	1.1	37
80	Design of ternary alkaline-earth metal Sn(<scp>ii</scp>) oxides with potential good p-type conductivity. Journal of Materials Chemistry C, 2016, 4, 4592-4599.	2.7	29
81	Chemical instability leads to unusual chemical-potential-independent defect formation and diffusion in perovskite solar cell material CH₃NH₃PbI₃. Journal of Materials Chemistry A, 2016, 4, 16975-16981.	5.2	67
82	Large dielectric constant, high acceptor density, and deep electron traps in perovskite solar cell material CsGeI₃. Journal of Materials Chemistry A, 2016, 4, 13852-13858.	5.2	148
83	Bismuth chalcohalides and oxyhalides as optoelectronic materials. Physical Review B, 2016, 93, .	1.1	82
84	Scintillation Properties and Electronic Structures of the Intrinsic and Extrinsic Mixed Elpasolites<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Cs</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub><mml:mrow><mml:mi mathvariant="normal">I</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mm. Physical Review Applied, 2016, 5, .	1.5	12
85	Observation of Nanoscale Morphological and Structural Degradation in Perovskite Solar Cells by in Situ TEM. ACS Applied Materials & Interfaces, 2016, 8, 32333-32340.	4.0	54
86	First-Principles Prediction of Thermodynamically Stable Two-Dimensional Electrides. Journal of the American Chemical Society, 2016, 138, 15336-15344.	6.6	91
87	Fast Diffusion of Native Defects and Impurities in Perovskite Solar Cell Material CH₃NH₃PbI₃. Chemistry of Materials, 2016, 28, 4349-4357.	3.2	139
88	Deciphering Halogen Competition in Organometallic Halide Perovskite Growth. Journal of the American Chemical Society, 2016, 138, 5028-5035.	6.6	92
89	Using DFT Methods to Study Activators in Optical Materials. ECS Journal of Solid State Science and Technology, 2016, 5, R3007-R3018.	0.9	31
90	Discrete Electronic Bands in Semiconductors and Insulators: Potential High-Light-Yield Scintillators. Physical Review Applied, 2015, 3, .	1.5	51

#	Article	IF	Citations
91	Li2Se:Te as a neutron scintillator. Journal of Alloys and Compounds, 2015, 647, 906-910.	2.8	7
92	Connecting Thermoelectric Performance and Topological-Insulator Behavior:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Bi</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mm xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Bi</mml:mi></mml:mrow><mml:m . Physical Review Applied, 2015, 3, .	1.5	178
93	Chemical stability and Ce doping of LiMgAlF6 neutron scintillator. Journal of Alloys and Compounds, 2015, 622, 925-928.	2.8	2
94	Native defects in Tl6SI4: Density functional calculations. Journal of Applied Physics, 2015, 117, .	1.1	7
95	Density Functional Calculations of Native Defects in CH₃NH₃PbI₃: Effects of Spinâ€“Orbit Coupling and Self-Interaction Error. Journal of Physical Chemistry Letters, 2015, 6, 1461-1466.	2.1	301
96	Ba2TeO as an optoelectronic material: First-principles study. Journal of Applied Physics, 2015, 117, 195705.	1.1	3
97	Crystal structure, electronic structure, temperature-dependent optical and scintillation properties of CsCe₂Br₇. Journal of Materials Chemistry C, 2015, 3, 11366-11376.	2.7	14
98	Mn4+ emission in pyrochlore oxides. Journal of Luminescence, 2015, 157, 69-73.	1.5	35
99	Shallow halogen vacancies in halide optoelectronic materials. Physical Review B, 2014, 90, .	1.1	119
100	Ternary chalcogenides<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:msub><mml:mi mathvariant="normal">s</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">Z</mml:mi><mml:msub><mml:mi mathvariant="normal">n</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mi mathvariant="normal">	1.1	9
101	Structural and crystal chemical properties of rare-earth titanate pyrochlores. Journal of Alloys and Compounds, 2014, 605, 63-70.	2.8	90
102	Chemical trends of Mn⁴⁺emission in solids. Journal of Materials Chemistry C, 2014, 2, 2475-2481.	2.7	214
103	Efficient carrier transport in halide perovskites: theoretical perspectives. Journal of Materials Chemistry A, 2014, 2, 9091-9098.	5.2	414
104	Chemical trends of electronic and optical properties of ns² ions in halides. Journal of Materials Chemistry C, 2014, 2, 4784-4791.	2.7	26
105	Identification of oxygen defects in CdTe revisited: First-principles study. Journal of Applied Physics, 2014, 115, 203511.	1.1	5
106	First principles calculations of Hydrogenâ€”Titanium vacancy complexes in SrTiO3. Ceramics International, 2013, 39, S273-S276.	2.3	4
107	Electronic structure engineering of elpasolites: Case of Cs2AgYCl6. Journal of Luminescence, 2013, 143, 710-714.	1.5	22
108	First-principles study of electronic structure, defects, and activators in LiCaAlF6. , 2013, , .		1

#	Article	IF	Citations
109	Effects of impurity doping on ionic conductivity and polarization phenomenon in TlBr. Applied Physics Letters, 2013, 102, 082102.	1.5	8
110	Potential thermoelectric performance of hole-doped Cu₂O. New Journal of Physics, 2013, 15, 043029.	1.2	47
111	High magnetocrystalline anisotropy in oxides with near cubic local environments. Applied Physics Letters, 2013, 102, .	1.5	6
112	Resistivity, carrier trapping, and polarization phenomenon in semiconductor radiation detection materials. Proceedings of SPIE, 2012, , .	0.8	6
113	Electronic structure, energy transport, and optical properties of halide scintillators. Proceedings of SPIE, 2012, , .	0.8	4
114	Energy transport and scintillation of cerium-doped elpasolite Cs<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>LiYCl<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>6</mml:mn></mml:msub></mml:math>: Hybrid density functional calculations. Physical Review B, 2012, 86, .	1.1	78
115	Electronic structure, small polaron, and F center in LiCaAlF6. Journal of Applied Physics, 2012, 112, 123516.	1.1	11
116	First-principles study of impurities in TlBr. Journal of Applied Physics, 2012, 111, 073519.	1.1	5
117	Electronic structure and defect properties of Tl<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>6</mml:mn></mml:msub></mml:math>SeI<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>: Density functional calculations. Physical Review B, 2012, 86, .	1.1	28
118	First principles study of O defects in CdSe. Physica B: Condensed Matter, 2012, 407, 2841-2845.	1.3	9
119	What causes high resistivity in CdTe. New Journal of Physics, 2012, 14, 063020.	1.2	57
120	Doping dependence of thermoelectric performance in Mo<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>Sb<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>7</mml:mn></mml:mro	1.1	21
121	Determination of miscibility in MgO-ZnO nanocrystal alloys by x-ray absorption spectroscopy. Applied Physics Letters, 2011, 99, 261901.	1.5	23
122	Spin Ice: Magnetic Excitations without Monopole Signatures Using Muon Spin Rotation. Physical Review Letters, 2011, 107, 207207.	2.9	60
123	Transport and optical properties of heavily hole-doped semiconductors BaCu2Se2 and BaCu2Te2. Journal of Solid State Chemistry, 2011, 184, 2744-2750.	1.4	25
124	Giant anharmonic phonon scattering in PbTe. Nature Materials, 2011, 10, 614-619.	13.3	561
125	Anionic and Hidden Hydrogen in ZnO. Physical Review Letters, 2011, 106, 115502.	2.9	84
126	First principles study of native defects in InI. Journal of Applied Physics, 2011, 109, 113518.	1.1	17

#	Article	IF	Citations
127	AX centers in II-VI semiconductors: Hybrid functional calculations. Applied Physics Letters, 2011, 98, .	1.5	18
128	First-principles Study of Back Contact Effects on CdTe Thin Film Solar Cells. Materials Research Society Symposia Proceedings, 2010, 1268, 1.	0.1	0
129	Enhanced Born charge and proximity to ferroelectricity in thallium halides. Physical Review B, 2010, 81, .	1.1	72
130	Enhanced Born charges in III-VII,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>IV-VII</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:m and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>V-VII</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:ms Physical Review B, 2010, 82, .	1.1	40
131	Properties of alkaline-earth-filled skutterudite antimonides:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

#	Article	IF	Citations
145	Native defects and oxygen and hydrogen-related defect complexes in CdTe: Density functional calculations. Journal of Applied Physics, 2008, 104, 093521.	1.1	50
146	Bismuth-induced deep levels and carrier compensation in CdTe. Physical Review B, 2008, 78, .	1.1	13
147	Trapped-Dopant Model of Doping in Semiconductor Nanocrystals. Nano Letters, 2008, 8, 2878-2882.	4.5	69
148	Electronic Structure, Magnetism and Spin-Fluctuations in Fe-As Based Superconductors. Materials Research Society Symposia Proceedings, 2008, 1148, 1.	0.1	0
149	Stabilization mechanisms of polar surfaces: ZnO surfaces. Physical Review B, 2008, 78, .	1.1	37
150	DX centers in CdTe: A density functional study. Applied Physics Letters, 2008, 92, 181908.	1.5	10
151	Carrier compensation in semi-insulating CdTe: First-principles calculations. Physical Review B, 2008, 77, .	1.1	59
152	Photo-Oxidation of Polyhydroxyl Molecules onTiO2Surfaces: From Hole Scavenging to Light-Induced Self-Assembly ofTiO2-Cyclodextrin Wires. Physical Review Letters, 2007, 98, 066102.	2.9	50
153	Unifying Chemical Bonding Models for Boranes. Materials Research Society Symposia Proceedings, 2007, 1038, 1.	0.1	1
154	First-principles study of native defects in anataseTiO2. Physical Review B, 2006, 73, .	1.1	346
155	Bistability-Mediated Carrier Recombination at Light-Induced Boron-Oxygen Complexes in Silicon. Physical Review Letters, 2006, 97, 256602.	2.9	35
156	Ion relaxation and hydrogen LVM in H-irradiated GaAsN. Physica B: Condensed Matter, 2006, 376-377, 583-586.	1.3	2
157	Quantum, classical, and multi-scale simulation of silicaâ€“water interaction: molecules, clusters, and extended systems. Journal of Computer-Aided Materials Design, 2006, 13, 161-183.	0.7	11
158	Hydrogen-Mediated Nitrogen Clustering in Dilute III-V Nitrides. Physical Review Letters, 2006, 97, 075503.	2.9	13
159	Hydrogen pairs and local vibrational frequencies in H-irradiatedGaAs1âˆ’yNy. Physical Review B, 2005, 72, .	1.1	33
160	Topological defects and the Staebler-Wronski effect in hydrogenated amorphous silicon. Applied Physics Letters, 2005, 87, 191903.	1.5	12
161	DXcenters in GaAs and GaSb. Physical Review B, 2005, 72, .	1.1	25
162	First-Principles Prediction of Icosahedral Quantum Dots for Tetravalent Semiconductors. Physical Review Letters, 2004, 93, .	2.9	55

#	Article	IF	Citations
163	Hydrolysis of a two-membered silica ring on the amorphous silica surface. Journal of Chemical Physics, 2004, 120, 1044-1054.	1.2	53
164	Coherent Electron Transport through an Azobenzene Molecule: A Light-Driven Molecular Switch. Physical Review Letters, 2004, 92, 158301.	2.9	249
165	Transparent interface between classical molecular dynamics and first-principles molecular dynamics. International Journal of Quantum Chemistry, 2003, 93, 1-8.	1.0	16
166	Bulk Separative Enrichment in Metallic or Semiconducting Single-Walled Carbon Nanotubes. Nano Letters, 2003, 3, 1245-1249.	4.5	246
167	Waterâ€“silica surface interactions: A combined quantum-classical molecular dynamic study of energetics and reaction pathways. Journal of Chemical Physics, 2003, 119, 6418-6422.	1.2	78
168	Manipulation of fullerene-induced impurity states in carbon peapods. Physical Review B, 2003, 68, .	1.1	25
169	Crossover in energy redistribution duringC60@Xe144surface impact. Physical Review B, 2001, 64, .	1.1	1