Meng-Qiu Cai

List of Publications by Year
in descending order

93 papers	3,168 citations	117571 34 h-index	182361 51 g-index
95 all docs	95 docs citations	95 times ranked	2823 citing authors

#	Article	IF	Citations
1	Layer-dependent transport and optoelectronic property in two-dimensional perovskite: (PEA)₂PbI₄. Nanoscale, 2018, 10, 8677-8688.	2.8	169
2	Boosted Photocatalytic Oxidation of Toluene into Benzaldehyde on CdIn₂S₄-CdS: Synergetic Effect of Compact Heterojunction and S-Vacancy. ACS Catalysis, 2021, 11, 2492-2503.	5.5	136
3	First-principles study on the electronic and optical properties of BiFeO3. Solid State Communications, 2009, 149, 641-644.	0.9	123
4	Interfacial charge behavior modulation in 2D/3D perovskite heterostructure for potential high-performance solar cells. Nano Energy, 2019, 59, 715-720.	8.2	108
5	Strong ferroelectric polarization of CH₃NH₃GeI₃ with high-absorption and mobility transport anisotropy: theoretical study. Journal of Materials Chemistry C, 2017, 5, 5356-5364.	2.7	101
6	Geometric structure and photovoltaic properties of mixed halide germanium perovskites from theoretical view. Organic Electronics, 2018, 53, 50-56.	1.4	74
7	Pressure-induced strong ferroelectric polarization in tetra-phase perovskite CsPbBr₃. Physical Chemistry Chemical Physics, 2018, 20, 14718-14724.	1.3	71
8	First-principles investigation of the Schottky contact for the two-dimensional MoS₂ and graphene heterostructure. RSC Advances, 2016, 6, 60271-60276.	1.7	68
9	Interface engineering of CsPbI3-black phosphorus van der Waals heterostructure. Applied Physics Letters, 2018, 112, .	1.5	67
10	Density functional theory calculation on two-dimensional MoS2/BiOX (Xâ€¯=â€¯Cl, Br, I) van der Waals heterostructures for photocatalytic action. Applied Surface Science, 2019, 492, 157-165.	3.1	65
11	A first-principles study of magnetic variation via doping vacancy in monolayer VS2. Journal of Magnetism and Magnetic Materials, 2016, 420, 218-224.	1.0	64
12	Density functional theory calculation on facet-dependent photocatalytic activity of MoS2/CdS heterostructures. Applied Surface Science, 2019, 469, 27-33.	3.1	63
13	Tuning the Schottky contacts in the phosphorene and graphene heterostructure by applying strain. Physical Chemistry Chemical Physics, 2016, 18, 19918-19925.	1.3	62
14	Strong thickness-dependent quantum confinement in all-inorganic perovskite Cs₂PbI₄with a Ruddlesdenâ€“Popper structure. Journal of Materials Chemistry C, 2019, 7, 7433-7441.	2.7	62
15	First-principles study of structural, electronic, and multiferroic properties in BiCoO3. Journal of Chemical Physics, 2007, 126, 154708.	1.2	60
16	First-principles hybrid functional study of the electronic structure and charge carrier mobility in perovskite CH ₃ NH ₃ SnI ₃. Chinese Physics B, 2016, 25, 107202.	0.7	56
17	Tuning Charge Carrier Types, Superior Mobility and Absorption in Lead-free Perovskite CH3NH3GeI3: Theoretical Study. Electrochimica Acta, 2017, 247, 891-898.	2.6	56
18	Layer-dependent optoelectronic property for all-inorganic two-dimensional mixed halide perovskite Cs2PbI2Cl2 with a Ruddlesden-Popper structure. Journal of Power Sources, 2020, 451, 227732.	4.0	55

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19	Magnetoelectric effect and critical thickness for ferroelectricity in Co/BaTiO3/Co multiferroic tunnel junctions. Journal of Applied Physics, 2011, 109, .	1.1	53
20	First-principles study of photovoltaics and carrier mobility for non-toxic halide perovskite CH₃NH₃SnCl₃: theoretical prediction. Physical Chemistry Chemical Physics, 2016, 18, 22188-22195.	1.3	53
21	Tuning superior solar cell performance of carrier mobility and absorption in perovskite CH 3 NH 3 GeCl 3 : A density functional calculations. Journal of Power Sources, 2016, 313, 96-103.	4.0	51
22	Oriented tuning the photovoltaic properties ofÎ³-RbGeX₃by strain-induced electron effective mass mutation. Journal Physics D: Applied Physics, 2017, 50, 465101.	1.3	50
23	Surface Terminationâ€"A Key Factor to Influence Electronic and Optical Properties of CsSnI3. Journal of Physical Chemistry C, 2018, 122, 9275-9282.	1.5	50
24	Two-Dimensional van der Waals Heterostructures Constructed via Perovskite (C₄H₉NH₃)₂XBr₄ and Black Phosphorus. Journal of Physical Chemistry Letters, 2018, 9, 4822-4827.	2.1	50
25	First-principles study of electronic and magnetic properties in Co doped BaTiO3. European Physical Journal B, 2015, 88, 1.	0.6	47
26	High-performance Photodetector Based on <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mrow><mml:mi>In</mml:mi><mml:mi>Se</mml:mi></mml:mrow><mml:mo>/</mml:mo><mml:msub><mml:m mathvariant="normal">I</mml:mi></mml:mrow></mml:mrow><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi>Cl</mml:mi>		

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37	Exploring the Coexistence Mechanism of CsPb₂Br₅ and CsPbBr₃ Based on the Competitive Phase Diagram. Journal of Physical Chemistry C, 2020, 124, 23052-23058.	1.5	35
38	Vanishing critical thickness in asymmetric ferroelectric tunnel junctions: First principle simulations. Journal of Applied Physics, 2011, 109, .	1.1	34
39	Tuning the Schottky rectification in graphene-hexagonal boron nitride-molybdenum disulfide heterostructure. Journal of Colloid and Interface Science, 2018, 513, 677-683.	5.0	34
40	Interfacial Interactions and Enhanced Optoelectronic Properties in CsSnI 3 â€“Black Phosphorus van der Waals Heterostructures. Physica Status Solidi (B): Basic Research, 2019, 256, 1800540.	0.7	34
41	Theoretical study on the intrinsic properties of In2Se3/MoS2 as a photocatalyst driven by near-infrared, visible and ultraviolet light. Catalysis Science and Technology, 2019, 9, 4659-4667.	2.1	31
42	Ni3S2@S-carbon nanotubes synthesized using NiS2 as sulfur source and precursor for high performance sodium-ion half/full cells. Science China Materials, 2020, 63, 216-228.	3.5	31
43	Vacancy-induced magnetism in BaTiO3(001) thin films based on density functional theory. Physical Chemistry Chemical Physics, 2011, 13, 4738.	1.3	29
44	ZnO-carbon nanofibers for stable, high response, and selective H₂S sensors. Nanotechnology, 2018, 29, 275501.	1.3	29
45	Theoretical prediction of double perovskite Cs₂Ag_xCu_{1-x}In_yTb_{1-y}Cl₆ for infrared detection. Journal Physics D: Applied Physics, 2020, 53, 265302.	1.3	29
46	Effects of composition modulation on the type of band alignments for Pd2Se3/CsSnBr3 van der waals heterostructure: A transition from type I to type II. Journal of Power Sources, 2020, 478, 229078.	4.0	27
47	Theoretical study on the effect of the optical properties and electronic structure for the Bi-doped CsPbBr₃. Journal of Physics Condensed Matter, 2020, 32, 205504.	0.7	27
48	Ab initio study of structural and electronic properties of SrTiO3 (001) oxygen-vacancy surfaces. Journal of Chemical Physics, 2006, 124, 174701.	1.2	26
49	Effect of grain boundaries on shock-induced phase transformation in iron bicrystals. Journal of Applied Physics, 2018, 123, .	1.1	25
50	Effects of Components Modulation on the Type of Band Alignments for PbI 2 /WS 2 van der Waals Heterostructure. Physica Status Solidi - Rapid Research Letters, 2020, 14, 2000016.	1.2	23
51	Effective shape-controlled synthesis of gallium selenide nanosheets by vapor phase deposition. Nano Research, 2020, 13, 557-563.	5.8	22
52	The influence of electrode for electroluminescence devices based on all-inorganic halide perovskite CsPbBr₃. Journal of Physics Condensed Matter, 2020, 32, 065002.	0.7	21
53	The energy band engineering for the high-performance infrared photodetectors constructed by CdTe/MoS₂ heterojunction. Journal of Physics Condensed Matter, 2020, 32, 065004.	0.7	20
54	Designing gâ€C₃N₄/Nâ€Rich Carbon Fiber Composites for Highâ€Performance Potassiumâ€Ion Hybrid Capacitors. Energy and Environmental Materials, 2021, 4, 638-645.	7.3	20

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55	Transition of the Type of Band Alignments for All-Inorganic Perovskite van der Waals Heterostructures CsSnBr₃/WS_{2(1â€“x)}Se_{2x}. Journal of Physical Chemistry Letters, 2021, 12, 3809-3818.	2.1	20
56	Tuning the Band Alignment and Electronic Properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mrow><mml:mi>Ga</mml:mi><mml:mi>Se</mml:mi></mml:mrow><mml:mo>/</mml:mo><mml:mi>Sn</mml:mi><mml:r X <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"		

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73	First-principles study on photovoltaic properties of 2D Cs₂PbI₄-black phosphorus heterojunctions. Journal of Physics Condensed Matter, 2020, 32, 195501.	0.7	10
74	Band alignment engineering of a Ruddlesdenâ€“Popper perovskite-based heterostructure constructed using Cs2SnI2Cl2 and Î±-In2Se3: The effects of ferroelectric polarization switching and electric fields. Applied Physics Letters, 2021, 119, 182903.	1.5	10
75	Dynamics of chiral domain wall under the spin-orbit torques in heavy metal/ferromagnet bilayers with in-plane anisotropy. Journal of Magnetism and Magnetic Materials, 2017, 441, 691-695.	1.0	9
76	Effects of Halogen Substitution on the Optoelectronic Properties of Two-Dimensional All-Inorganic Double Perovskite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mi>Cs</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:mrow><mml:mi>Ag</mml:mi><mml:mi		

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91	2D and 3D double perovskite with dimensionality-dependent optoelectronic properties: first-principle study on Cs₂AgBiBr₆ and Cs₄AgBiBr₈. Journal of Physics Condensed Matter, 2022, 34, 065501.	0.7	3
92	Walker solution for a magnetic domain wall driven by spin-orbit torques. Physical Review B, 2020, 102, .	1.1	3
93	First principles prediction of the carrier mobilities and optical properties of strained lead free perovskite Cs2SnX6(X=Cl, Br). Solid State Communications, 2022, 353, 114868.	0.9	0