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	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
2	Origami-controlled strain engineering of tunable flat bands and correlated states in folded graphene. Physical Review Materials, 2022, 6, .	0.9	9
3	Restricting the Formation of Pbâ€“Pb Dimer via Surface Pb Site Passivation for Enhancing the Light Stability of Perovskite. Small, 2022, 18, e2201831.	5.2	15
4	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
5	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
6	High-performance photovoltaic application of the 2D all-inorganic Ruddlesdenâ€“Popper perovskite heterostructure Cs₂PbI₂Cl₂/MAPbI₃. Physical Chemistry Chemical Physics, 2021, 23, 23703-23710.	1.3	6
7	Controllable deposition of FeV2S4 in carbon fibers for sodium-ion storage with high capacity and long lifetime. Science China Materials, 2021, 64, 1355-1366.	3.5	15
8	Enhanced photocatalytic activity of the direct Z-scheme black phosphorus/BiOX (X = Cl, Br, I) heterostructures. Physical Chemistry Chemical Physics, 2021, 23, 17894-17903.	1.3	19
9	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
10	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
11	Structural, electronic, and charge transfer features for two kinds of MoS2/Cs2PbI4 interfaces with optoelectronic applicability: Insights from first-principles. Applied Physics Letters, 2021, 118, .	1.5	4
12	Photocatalytic Nitrogen Reduction Reaction over Two-Dimensional Cs₃Bi₂Br₉â€“CdS Van der Waals Heterostructures by External Control Strategies. Journal of Physical Chemistry C, 2021, 125, 13212-13224.	1.5	8
13	Effects of component on the photoelectric properties of two-dimensional van der Waals heterostructure Cs₂PbI_{2(1+x)}Cl_{2(1â^’x)}/Pd₂Se₃ with Ruddlesenâ€“Popper structure. Journal Physics D: Applied Physics, 2021, 54, 355110.	1.3	4
14	Theoretical study on the tunable electronic band structure of Cs2PbI2Cl2/CsPbBr3 halide perovskite heterostructure driven by ferroelectric polarization modulation. Journal of Colloid and Interface Science, 2021, 597, 233-241.	5.0	14
15	Synthesis of ultrathin PdSe2 flakes for hydrogen evolution reaction. Applied Surface Science, 2021, 570, 151178.	3.1	11
16	Effects of doping on photocatalytic water splitting activities of PtS₂/SnS₂ van der Waals heterostructures. Physical Chemistry Chemical Physics, 2021, 23, 18125-18136.	1.3	17
17	Thickness-induced band-gap engineering in lead-free double perovskite Cs₂AgBiBr₆ for highly efficient photocatalysis. Physical Chemistry Chemical Physics, 2021, 23, 12439-12445.	1.3	14
18	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:m X <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"		

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19	Equilibria and precession in a uniaxial antiferromagnet driven by the spin Hall effect. New Journal of Physics, 2021, 23, 113020.	1.2	4
20	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
21	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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37	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
38	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
39	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
40	Interfacial electronic properties of 2D/3D (PtSe₂/CsPbX₃) perovskite heterostructure. Journal of Physics Condensed Matter, 2020, 32, 445004.	0.7	4
41	Walker solution for a magnetic domain wall driven by spin-orbit torques. Physical Review B, 2020, 102, .	1.1	3
42	Interactions of plasticity and phase transformation under shock in iron bicrystals. Journal of Applied Physics, 2019, 126, .	1.1	7
43	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
44	Breaking the anisotropy of Î±-CNH and improving the photoelectric performance by constructing Van der Waals heterojunction. Applied Surface Science, 2019, 497, 143787.	3.1	17
45	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
46	First-principles investigations of electronic and optical properties in the MoS2/CsPbBr3 heterostructure. Journal of Physics and Chemistry of Solids, 2019, 135, 109060.	1.9	39
47	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
48	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
49	Interfacial charge behavior modulation in 2D/3D perovskite heterostructure for potential high-performance solar cells. Nano Energy, 2019, 59, 715-720.	8.2	108
50	Motion and stability of chiral domain walls driven by non-gradient spin torques: Antiferromagnets and ferromagnets compared. Journal of Magnetism and Magnetic Materials, 2019, 479, 291-300.	1.0	3
51	Density functional theory calculation on facet-dependent photocatalytic activity of MoS2/CdS heterostructures. Applied Surface Science, 2019, 469, 27-33.	3.1	63
52	Theoretical study on photoelectric properties of lead-free mixed inorganic perovskite RbGe1-xSnxI3. Current Applied Physics, 2019, 19, 279-284.	1.1	42
53	High transport and excellent optical property of a two-dimensional single-layered hybrid perovskite (C₄H₉NH₃)₂PbBr₄: a theoretical study. Physical Chemistry Chemical Physics, 2018, 20, 13241-13248.	1.3	17
54	Layer-dependent transport and optoelectronic property in two-dimensional perovskite: (PEA)₂PbI₄. Nanoscale, 2018, 10, 8677-8688.	2.8	169

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55	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
56	ZnO-carbon nanofibers for stable, high response, and selective H₂S sensors. Nanotechnology, 2018, 29, 275501.	1.3	29
57	Interface engineering of CsPbI3-black phosphorus van der Waals heterostructure. Applied Physics Letters, 2018, 112, .	1.5	67
58	Effect of grain boundaries on shock-induced phase transformation in iron bicrystals. Journal of Applied Physics, 2018, 123, .	1.1	25
59	Influence of the number of layers on ultrathin CsSnI₃ perovskite: from electronic structure to carrier mobility. Journal Physics D: Applied Physics, 2018, 51, 105101.	1.3	35
60	Pressure-induced strong ferroelectric polarization in tetra-phase perovskite CsPbBr₃. Physical Chemistry Chemical Physics, 2018, 20, 14718-14724.	1.3	71
61	Geometric structure and photovoltaic properties of mixed halide germanium perovskites from theoretical view. Organic Electronics, 2018, 53, 50-56.	1.4	74
62	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
63	Ferroelectric Polarization in CsPbI₃/CsSnI₃ Perovskite Heterostructure. Journal of Physical Chemistry C, 2018, 122, 17820-17824.	1.5	11
64	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
65	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
66	Role of electrodes materials in determining the interfacial and magnetoelectric properties in BaTiO3-based multiferroic tunnel junctions. European Physical Journal B, 2017, 90, 1.	0.6	14
67	Co₃O₄â€"SnO₂ nanobox sensor with a PN junction and semiconductorâ€"conductor transformation for high selectivity and sensitivity detection of H₂S. CrystEngComm, 2017, 19, 5742-5748.	1.3	35
68	Oriented tuning the photovoltaic properties ofÎ³-RbGeX₃by strain-induced electron effective mass mutation. Journal Physics D: Applied Physics, 2017, 50, 465101.	1.3	50
69	Tuning Charge Carrier Types, Superior Mobility and Absorption in Lead-free Perovskite CH3NH3GeI3: Theoretical Study. Electrochimica Acta, 2017, 247, 891-898.	2.6	56
70	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
71	In Situ Barbecue-Like Fabrication of Porous Ag/Fe2O3 Sensors. Nanoscience and Nanotechnology Letters, 2017, 9, 1387-1392.	0.4	3
72	Tuning the Schottky contacts in the phosphorene and graphene heterostructure by applying strain. Physical Chemistry Chemical Physics, 2016, 18, 19918-19925.	1.3	62

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73	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
74	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
75	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
76	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
77	First-principles investigation of the Schottky contact for the two-dimensional MoS₂ and graphene heterostructure. RSC Advances, 2016, 6, 60271-60276.	1.7	68
78	Interfacial structure, ferroelectric stability, and magnetoelectric effect of magnetoelectric junction FeCo/BaTiO3/FeCo with alloy electrode. Journal of Materials Science, 2016, 51, 3297-3302.	1.7	3
79	The interfacial properties of SrRuO3/MoS2 heterojunction: a first-principles study. European Physical Journal B, 2016, 89, 1.	0.6	41
80	First-principles study of electronic and magnetic properties in Co doped BaTiO3. European Physical Journal B, 2015, 88, 1.	0.6	47
81	Tuning the Schottky barrier height of the Pdâ€“MoS₂ contact by different strains. Physical Chemistry Chemical Physics, 2015, 17, 27088-27093.	1.3	40
82	Stability analysis of current-driven domain wall in the presence of spin Hall effect. Journal of Applied Physics, 2013, 114, .	1.1	8
83	Vacancy-induced magnetism in BaTiO3(001) thin films based on density functional theory. Physical Chemistry Chemical Physics, 2011, 13, 4738.	1.3	29
84	Effect of nitrogen doping on optical properties and electronic structures of SrZrO3 films. Solid State Communications, 2011, 151, 280-283.	0.9	14
85	Uniaxial strain-modulated conductivity in manganite superlattice (LaMnO3/SrMnO3). Applied Physics Letters, 2011, 98, 031910.	1.5	40
86	Magnetoelectric effect and critical thickness for ferroelectricity in Co/BaTiO3/Co multiferroic tunnel junctions. Journal of Applied Physics, 2011, 109, .	1.1	53
87	Vanishing critical thickness in asymmetric ferroelectric tunnel junctions: First principle simulations. Journal of Applied Physics, 2011, 109, .	1.1	34
88	First-principles study of the critical thickness in asymmetric ferroelectric tunnel junctions. Applied Physics Letters, 2011, 98, .	1.5	35
89	First-principles study on the electronic and optical properties of BiFeO3. Solid State Communications, 2009, 149, 641-644.	0.9	123
90	Joint experiment and theory to study the band structure of SrZrO3 in orthorhombic phase. Solid State Communications, 2009, 149, 2250-2253.	0.9	8

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91	First-principles study of structural, electronic, and multiferroic properties in BiCoO3. Journal of Chemical Physics, 2007, 126, 154708.	1.2	60
92	Ab initio study of structural and electronic properties of SrTiO3 (001) oxygen-vacancy surfaces. Journal of Chemical Physics, 2006, 124, 174701.	1.2	26
93	First-principles study of structural and electronic properties ofBaTiO3(001)oxygen-vacancy surfaces. Physical Review B, 2005, 72, .	1.1	44