

Meng-Qiu Cai

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/1472589/publications.pdf>

Version: 2024-02-01

93
papers

3,168
citations

134610

34
h-index

206121

51
g-index

95
all docs

95
docs citations

95
times ranked

3210
citing authors

#	ARTICLE	IF	CITATIONS
1	2D and 3D double perovskite with dimensionality-dependent optoelectronic properties: first-principle study on Cs ₂ AgBiBr ₆ and Cs ₄ AgBiBr ₈ . 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 Pb ²⁺ -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 Cs ₂ SnX ₆ (X=Cl, Br). Solid State Communications, 2022, 353, 114868.	0.9	0
5	Designing g ₃ N ₄ /N-Rich Carbon Fiber Composites for High-Performance Potassium-Ion Hybrid Capacitors. Energy and Environmental Materials, 2021, 4, 638-645.	7.3	20
6	High-performance photovoltaic application of the 2D all-inorganic Ruddlesden-Popper perovskite heterostructure Cs ₂ PbI ₂ Cl ₂ /MAPbI ₃ . Physical Chemistry Chemical Physics, 2021, 23, 23703-23710.	1.3	6
7	Controllable deposition of FeV ₂ S ₄ 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 CdIn ₂ S ₄ -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 CsSnBr ₃ /WS ₂ (1 ^x)Se ₂ (^x). Journal of Physical Chemistry Letters, 2021, 12, 3809-3818.	2.1	20
11	Structural, electronic, and charge transfer features for two kinds of MoS ₂ /Cs ₂ PbI ₄ interfaces with optoelectronic applicability: Insights from first-principles. Applied Physics Letters, 2021, 118, .	1.5	4
12	Photocatalytic Nitrogen Reduction Reaction over Two-Dimensional Cs ₃ Bi ₂ Br ₉ -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 Cs ₂ PbI ₂ (1+x)Cl ₂ (1-x)/Pd ₂ Se ₃ with Ruddlesden-Popper structure. Journal Physics D: Applied Physics, 2021, 54, 355110.	1.3	4
14	Theoretical study on the tunable electronic band structure of Cs ₂ PbI ₂ Cl ₂ /CsPbBr ₃ 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 PdSe ₂ flakes for hydrogen evolution reaction. Applied Surface Science, 2021, 570, 151178.	3.1	11
16	Effects of doping on photocatalytic water splitting activities of PtS ₂ /SnS ₂ 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 Cs ₂ AgBiBr ₆ for highly efficient photocatalysis. Physical Chemistry Chemical Physics, 2021, 23, 18125-18136.	1.3	14
18	Tuning the Band Alignment and Electronic Properties of GaSe/SnX_2		

#	ARTICLE	IF	CITATIONS
19	Equilibria and precession in a uniaxial antiferromagnet driven by the spin Hall effect. <i>New Journal of Physics</i> , 2021, 23, 113020.	1.2	4
20	Band alignment engineering of a Ruddlesden-Popper perovskite-based heterostructure constructed using Cs ₂ SnI ₂ Cl ₂ and \pm -In ₂ Se ₃ : The effects of ferroelectric polarization switching and electric fields. <i>Applied Physics Letters</i> , 2021, 119, 182903.	1.5	10
21	Effects of Halogen Substitution on the Optoelectronic Properties of Two-Dimensional All-Inorganic Double Perovskite $\text{Cs}_{4-x}\text{Ag}_x\text{M}_2\text{X}_8$		

#	ARTICLE	IF	CITATIONS
37	Layer-dependent optoelectronic property for all-inorganic two-dimensional mixed halide perovskite Cs ₂ PbI ₂ Cl ₂ 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 Pbl 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 Cs ₂ Ag _x Cu _{1-x} In _y Tb _{1-y} Cl ₆ for infrared detection. Journal Physics D: Applied Physics, 2020, 53, 265302.	1.3	29
40	Interfacial electronic properties of 2D/3D (PtSe ₂ /CsPbX ₃) 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 In ₂ Se ₃ /MoS ₂ 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 I±-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 MoS ₂ /BiOX (X=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 MoS ₂ /CsPbBr ₃ heterostructure. Journal of Physics and Chemistry of Solids, 2019, 135, 109060.	1.9	39
47	Strong thickness-dependent quantum confinement in all-inorganic perovskite Cs ₂ PbI ₄ with a Ruddlesden-Popper structure. Journal of Materials Chemistry C, 2019, 7, 7433-7441.	2.7	62
48	Interfacial Interactions and Enhanced Optoelectronic Properties in CsSnI ₃ "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 MoS ₂ /CdS heterostructures. Applied Surface Science, 2019, 469, 27-33.	3.1	63
52	Theoretical study on photoelectric properties of lead-free mixed inorganic perovskite RbGe _{1-x} Sn _x I ₃ . 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 (C ₄ H ₉ NH ₃) ₂ PbBr ₄ : 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) ₂ PbI ₄ . Nanoscale, 2018, 10, 8677-8688.	2.8	169

#	ARTICLE	IF	CITATIONS
55	Surface Terminationâ€”A Key Factor to Influence Electronic and Optical Properties of CsSnI ₃ . Journal of Physical Chemistry C, 2018, 122, 9275-9282.	1.5	50
56	ZnO-carbon nanofibers for stable, high response, and selective H ₂ S sensors. Nanotechnology, 2018, 29, 275501.	1.3	29
57	Interface engineering of CsPbI ₃ -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 CsSn ₃ 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 CsPbBr ₃ . 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 CsPb ₃ /CsSn ₃ Perovskite Heterostructure. Journal of Physical Chemistry C, 2018, 122, 17820-17824.	1.5	11
64	Two-Dimensional van der Waals Heterostructures Constructed via Perovskite (C ₄ H ₉ NH ₃) ₂ XBr ₄ and Black Phosphorus. Journal of Physical Chemistry Letters, 2018, 9, 4822-4827.	2.1	50
65	Strong ferroelectric polarization of CH ₃ NH ₃ Ge ₃ 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 BaTiO ₃ -based multiferroic tunnel junctions. European Physical Journal B, 2017, 90, 1.	0.6	14
67	Co ₃ O ₄ â€”SnO ₂ nanobox sensor with a PN junction and semiconductorâ€”conductor transformation for high selectivity and sensitivity detection of H ₂ S. CrystEngComm, 2017, 19, 5742-5748.	1.3	35
68	Oriented tuning the photovoltaic properties of ¹³⁷ RbGeX ₃ by 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 CH ₃ NH ₃ GeI ₃ : 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/Fe ₂ O ₃ 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

#	ARTICLE	IF	CITATIONS
73	First-principles study of photovoltaics and carrier mobility for non-toxic halide perovskite $\text{CH}_3\text{NH}_3\text{SnCl}_3$: theoretical prediction. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 22188-22195.	1.3	53
74	Tuning superior solar cell performance of carrier mobility and absorption in perovskite $\text{CH}_3\text{NH}_3\text{GeCl}_3$: A density functional calculations. <i>Journal of Power Sources</i> , 2016, 313, 96-103.	4.0	51
75	A first-principles study of magnetic variation via doping vacancy in monolayer VS_2 . <i>Journal of Magnetism and Magnetic Materials</i> , 2016, 420, 218-224.	1.0	64
76	First-principles hybrid functional study of the electronic structure and charge carrier mobility in perovskite $\text{CH}_3\text{NH}_3\text{SnI}_3$. <i>Chinese Physics B</i> , 2016, 25, 107202.	0.7	56
77	First-principles investigation of the Schottky contact for the two-dimensional MoS_2 and graphene heterostructure. <i>RSC Advances</i> , 2016, 6, 60271-60276.	1.7	68
78	Interfacial structure, ferroelectric stability, and magnetoelectric effect of magnetoelectric junction $\text{FeCo}/\text{BaTiO}_3/\text{FeCo}$ with alloy electrode. <i>Journal of Materials Science</i> , 2016, 51, 3297-3302.	1.7	3
79	The interfacial properties of $\text{SrRuO}_3/\text{MoS}_2$ heterojunction: a first-principles study. <i>European Physical Journal B</i> , 2016, 89, 1.	0.6	41
80	First-principles study of electronic and magnetic properties in Co doped BaTiO_3 . <i>European Physical Journal B</i> , 2015, 88, 1.	0.6	47
81	Tuning the Schottky barrier height of the Pd/MoS_2 contact by different strains. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 27088-27093.	1.3	40
82	Stability analysis of current-driven domain wall in the presence of spin Hall effect. <i>Journal of Applied Physics</i> , 2013, 114, .	1.1	8
83	Vacancy-induced magnetism in $\text{BaTiO}_3(001)$ thin films based on density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 4738.	1.3	29
84	Effect of nitrogen doping on optical properties and electronic structures of SrZrO_3 films. <i>Solid State Communications</i> , 2011, 151, 280-283.	0.9	14
85	Uniaxial strain-modulated conductivity in manganite superlattice ($\text{LaMnO}_3/\text{SrMnO}_3$). <i>Applied Physics Letters</i> , 2011, 98, 031910.	1.5	40
86	Magnetoelectric effect and critical thickness for ferroelectricity in $\text{Co}/\text{BaTiO}_3/\text{Co}$ multiferroic tunnel junctions. <i>Journal of Applied Physics</i> , 2011, 109, .	1.1	53
87	Vanishing critical thickness in asymmetric ferroelectric tunnel junctions: First principle simulations. <i>Journal of Applied Physics</i> , 2011, 109, .	1.1	34
88	First-principles study of the critical thickness in asymmetric ferroelectric tunnel junctions. <i>Applied Physics Letters</i> , 2011, 98, .	1.5	35
89	First-principles study on the electronic and optical properties of BiFeO_3 . <i>Solid State Communications</i> , 2009, 149, 641-644.	0.9	123
90	Joint experiment and theory to study the band structure of SrZrO_3 in orthorhombic phase. <i>Solid State Communications</i> , 2009, 149, 2250-2253.	0.9	8

#	ARTICLE	IF	CITATIONS
91	First-principles study of structural, electronic, and multiferroic properties in BiCoO ₃ . Journal of Chemical Physics, 2007, 126, 154708.	1.2	60
92	Ab initio study of structural and electronic properties of SrTiO ₃ (001) oxygen-vacancy surfaces. Journal of Chemical Physics, 2006, 124, 174701.	1.2	26
93	First-principles study of structural and electronic properties of BaTiO ₃ (001) oxygen-vacancy surfaces. Physical Review B, 2005, 72, .	1.1	44