Shi Liu

List of Publications by Year
in descending order

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65	3,673	147726 31	128225 60
papers	citations	h-index	g-index

66	66	66	5980
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Rashba Spinâ€“Orbit Coupling Enhanced Carrier Lifetime in CH₃NH₃PbI₃. Nano Letters, 2015, 15, 7794-7800.	4.5	438
2	Ferroelectric Domain Wall Induced Band Gap Reduction and Charge Separation in Organometal Halide Perovskites. Journal of Physical Chemistry Letters, 2015, 6, 693-699.	2.1	293
3	High Chloride Doping Levels Stabilize the Perovskite Phase of Cesium Lead Iodide. Nano Letters, 2016, 16, 3563-3570.	4.5	247
4	Shift current bulk photovoltaic effect in polar materialsâ€”hybrid and oxide perovskites and beyond. Npj Computational Materials, 2016, 2, .	3.5	246
5	Ferroelectric polarization reversal via successive ferroelastic transitions. Nature Materials, 2015, 14, 79-86.	13.3	216
6	Slush-like polar structures in single-crystal relaxors. Nature, 2017, 546, 391-395.	13.7	201
7	Intrinsic ferroelectric switching from first principles. Nature, 2016, 534, 360-363.	13.7	151
8	Light-induced picosecond rotational disordering of the inorganic sublattice in hybrid perovskites. Science Advances, 2017, 3, e1602388.	4.7	149
9	Strain-induced room-temperature ferroelectricity in SrTiO3 membranes. Nature Communications, 2020, 11, 3141.	5.8	121
10	Polarization Dependence of Water Adsorption to CH₃NH₃PbI₃ (001) Surfaces. Journal of Physical Chemistry Letters, 2015, 6, 4371-4378.	2.1	111
11	Strain-Induced Ferroelectric Topological Insulator. Nano Letters, 2016, 16, 1663-1668.	4.5	82
12	Resonant domain-wall-enhanced tunable microwave ferroelectrics. Nature, 2018, 560, 622-627.	13.7	82
13	Ultrafast terahertz-field-driven ionic response in ferroelectric <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">BaTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2016, 94, .	1.1	78
14	Photoferroelectric and Photopiezoelectric Properties of Organometal Halide Perovskites. Journal of Physical Chemistry Letters, 2016, 7, 1460-1465.	2.1	73
15	Origin of Negative Longitudinal Piezoelectric Effect. Physical Review Letters, 2017, 119, 207601.	2.9	63
16	Large polarization gradients and temperature-stable responses in compositionally-graded ferroelectrics. Nature Communications, 2017, 8, 14961.	5.8	60
17	Effects of growth orientations and epitaxial strains on phase stability of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>HfO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> thin films. Physical Review Materials, 2019, 3, .	0.9	58
18	Atomistic description for temperature-driven phase transitions in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> Physical Review B, 2016, 94, .	1.1	52

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19	Reinterpretation of the bond-valence model with bond-order formalism: An improved bond-valence-based interatomic potential for PbTiO<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>. Physical Review B, 2013, 88, .	1.1	50
20	Development of a bond-valence based interatomic potential for BiFeO₃for accurate molecular dynamics simulations. Journal of Physics Condensed Matter, 2013, 25, 102202.	0.7	47
21	Ultrafast Terahertz Gating of the Polarization and Giant Nonlinear Optical Response in BiFeO₃ Thin Films. Advanced Materials, 2015, 27, 6371-6375.	11.1	47
22	Kinetic control of tunable multi-state switching in ferroelectric thin films. Nature Communications, 2019, 10, 1282.	5.8	47
23	Effect of Microphase Separation on the Protein Resistance of a Polymeric Surface. Langmuir, 2009, 25, 9467-9472.	1.6	40
24	Deep learning of accurate force field of ferroelectric <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>HfO</mml:mi></mml:mrow><mml:mn>2</m Physical Review B, 2021, 103, .	1.1	39
25	Backbiting and Î²-scission reactions in free-radical polymerization of methyl acrylate. International Journal of Quantum Chemistry, 2014, 114, 345-360.	1.0	38
26	Material Innovation in Advancing Organometal Halide Perovskite Functionality. Journal of Physical Chemistry Letters, 2015, 6, 4862-4872.	2.1	37
27	Origin of Pyroelectricity in Ferroelectric HfO ₂. Physical Review Applied, 2019, 12, .	1.5	37
28	Ferroelectric structural transition in hafnium oxide induced by charged oxygen vacancies. Physical Review B, 2021, 104, .	1.1	35
29	Modeling Spin-Forbidden Monomer Self-Initiation Reactions in Spontaneous Free-Radical Polymerization of Acrylates and Methacrylates. Journal of Physical Chemistry A, 2014, 118, 9310-9318.	1.1	34
30	Response of Methylammonium Lead Iodide to External Stimuli and Caloric Effects from Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2016, 120, 17274-17281.	1.5	33
31	Electric Auxetic Effect in Piezoelectrics. Physical Review Letters, 2020, 125, 197601.	2.9	32
32	Computational Study of Chain Transfer to Monomer Reactions in High-Temperature Polymerization of Alkyl Acrylates. Journal of Physical Chemistry A, 2013, 117, 2605-2618.	1.1	30
33	Strong Roomâ€Temperature Ferroelectricity in Strained SrTiO₃ Homoepitaxial Film. Advanced Materials, 2021, 33, e2008316.	11.1	28
34	Electron-beam-induced ferroelectric domain behavior in the transmission electron microscope: Toward deterministic domain patterning. Physical Review B, 2016, 94, .	1.1	26
35	T-square resistivity without Umklapp scattering in dilute metallic Bi2O2Se. Nature Communications, 2020, 11, 3846.	5.8	26
36	Structural phase transitions in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>SrTi</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> from deep potential molecular dynamics. Physical Review B, 2022, 105, .	1.1	25

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37	Computational Study of Cyclohexanoneâ€“Monomer Co-initiation Mechanism in Thermal Homo-polymerization of Methyl Acrylate and Methyl Methacrylate. Journal of Physical Chemistry A, 2012, 116, 5337-5348.	1.1	23
38	Ultrafast Electric Field Pulse Control of Giant Temperature Change in Ferroelectrics. Physical Review Letters, 2018, 120, 055901.	2.9	21
39	Theoretical Study of Intermolecular Chain Transfer to Polymer Reactions of Alkyl Acrylates. Industrial & Engineering Chemistry Research, 2015, 54, 4148-4165.	1.8	20
40	Asymmetry in mechanical polarization switching. Applied Physics Letters, 2017, 110, .	1.5	20
41	Accurate force field of two-dimensional ferroelectrics from deep learning. Physical Review B, 2021, 104, .	1.1	18
42	Multiscale simulations of defect dipoleâ€“enhanced electromechanical coupling at dilute defect concentrations. Applied Physics Letters, 2017, 111, .	1.5	17
43	Two-dimensional ferroelectric metal for electrocatalysis. Materials Horizons, 2021, 8, 3387-3393.	6.4	17
44	First-principles study of two-dimensional ferroelectrics using self-consistent Hubbard parameters. Physical Review B, 2020, 102, .	1.1	16
45	Giant Bulk Photovoltaic Effect in Vinylene-Linked Hybrid Heterocyclic Polymer. Journal of Physical Chemistry C, 2017, 121, 6500-6507.	1.5	15
46	Origin of stationary domain wall enhanced ferroelectric susceptibility. Physical Review B, 2017, 95, .	1.1	15
47	Exploration of the intrinsic inertial response of ferroelectric domain walls via molecular dynamics simulations. Applied Physics Letters, 2013, 103, .	1.5	13
48	A two-dimensional multiferroic metal with voltage-tunable magnetization and metallicity. Materials Horizons, 2021, 8, 2316-2324.	6.4	13
49	On-demand quantum spin Hall insulators controlled by two-dimensional ferroelectricity. Materials Horizons, 2022, 9, 1440-1447.	6.4	13
50	Combining inverse and conventional pyroelectricity in antiferroelectric thin films for energy conversion. Journal of Materials Chemistry C, 2018, 6, 9828-9834.	2.7	12
51	Asymmetric Response of Ferroelastic Domain-Wall Motion under Applied Bias. ACS Applied Materials & Interfaces, 2016, 8, 2935-2941.	4.0	11
52	The other model antiferroelectric: PbHfO3 thin films from ALD precursors. APL Materials, 2021, 9, .	2.2	11
53	Stable charged antiparallel domain walls in hyperferroelectrics. Journal of Physics Condensed Matter, 2017, 29, 244003.	0.7	10
54	Quantum pressure and chemical bonding: Influence of magnetic fields on electron localization. Physical Review B, 2015, 92, .	1.1	8

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55	Structure and properties of edge dislocations in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>BiFe</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, 2019, 3, .	0.9	7
56	Engineering Individual Oxygen Vacancies: Domain-Wall Conductivity and Controllable Topological Solitons. ACS Nano, 2021, 15, 13380-13388.	7.3	5
57	Multiscale Catalyst Design for Steam Methane Reforming Assisted by Deep Learning. Journal of Physical Chemistry C, 2021, 125, 10860-10867.	1.5	4
58	Oxygen-Initiated Free-Radical Polymerization of Alkyl Acrylates at High Temperatures. Macromolecules, 2021, 54, 7925-7930.	2.2	3
59	Extension of Snoekâ€™s Law to Higher RF Frequencies by Controlling Nanomagnetic Particle Parameters. , 2019, , .		2
60	Possible existence of tristable polarization states in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>LiNbO</mml:mi><mml:mn>3</mml:mn></mml:msub></m under an open-circuit boundary condition. Physical Review B, 2021, 104, .	1.1	2
61	Designing xenes with two-dimensional triangular lattice. Physical Review Materials, 2020, 4, .	0.9	2
62	Reply to â€œComment on â€˜Ultrafast terahertz-field-driven ionic response in ferroelectric <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></m ' â€• Physical Review B, 2018, 97, .	1.1	1
63	Alkali-metal induced electronic structure evolution in Sn4Sb3 studied by angle-resolved photoemission spectroscopy. Journal of Physics and Chemistry of Solids, 2022, 162, 110526.	1.9	1
64	Toward Deterministic Switching in Ferroelectric Systems: Insight Gained from In Situ TEM. Microscopy and Microanalysis, 2015, 21, 1347-1348.	0.2	0
65	Comment on â€œUltrafast terahertz-field-driven ionic response in ferroelectric BaTiO3 â€• Physical Review B, 2018, 97, .	1.1	0