Shi Liu

List of Publications by Year
in descending order

65 papers	3,673 citations	168829 31 h-index	145109 60 g-index
66 all docs	66 docs citations	66 times ranked	6950 citing authors

#	Article	IF	Citations
1	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
2	On-demand quantum spin Hall insulators controlled by two-dimensional ferroelectricity. Materials Horizons, 2022, 9, 1440-1447.	6.4	13
3	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
4	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</mml:mn></mml:msub></mml:math> Physical Review B, 2021, 103, .	1.1	39
5	Two-dimensional ferroelectric metal for electrocatalysis. Materials Horizons, 2021, 8, 3387-3393.	6.4	17
6	The other model antiferroelectric: PbHfO3 thin films from ALD precursors. APL Materials, 2021, 9, .	2.2	11
7	Strong Roomâ€Temperature Ferroelectricity in Strained SrTiO₃ Homoepitaxial Film. Advanced Materials, 2021, 33, e2008316.	11.1	28
8	Multiscale Catalyst Design for Steam Methane Reforming Assisted by Deep Learning. Journal of Physical Chemistry C, 2021, 125, 10860-10867.	1.5	4
9	Engineering Individual Oxygen Vacancies: Domain-Wall Conductivity and Controllable Topological Solitons. ACS Nano, 2021, 15, 13380-13388.	7.3	5
10	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></mml:mrow></mml:math> under an open-circuit boundary condition. Physical Review B, 2021, 104, .	1.1	2
11	Oxygen-Initiated Free-Radical Polymerization of Alkyl Acrylates at High Temperatures. Macromolecules, 2021, 54, 7925-7930.	2.2	3
12	A two-dimensional multiferroic metal with voltage-tunable magnetization and metallicity. Materials Horizons, 2021, 8, 2316-2324.	6.4	13
13	Accurate force field of two-dimensional ferroelectrics from deep learning. Physical Review B, 2021, 104, .	1.1	18
14	Ferroelectric structural transition in hafnium oxide induced by charged oxygen vacancies. Physical Review B, 2021, 104, .	1.1	35
15	T-square resistivity without Umklapp scattering in dilute metallic Bi2O2Se. Nature Communications, 2020, 11, 3846.	5.8	26
16	Electric Auxetic Effect in Piezoelectrics. Physical Review Letters, 2020, 125, 197601.	2.9	32
17	First-principles study of two-dimensional ferroelectrics using self-consistent Hubbard parameters. Physical Review B, 2020, 102, .	1.1	16
18	Strain-induced room-temperature ferroelectricity in SrTiO3 membranes. Nature Communications, 2020, 11, 3141.	5.8	121

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19	Designing xenes with two-dimensional triangular lattice. Physical Review Materials, 2020, 4, .	0.9	2
20	Origin of Pyroelectricity in Ferroelectric HfO ₂. Physical Review Applied, 2019, 12, .	1.5	37
21	Kinetic control of tunable multi-state switching in ferroelectric thin films. Nature Communications, 2019, 10, 1282.	5.8	47
22	Extension of Snoekâ€™s Law to Higher RF Frequencies by Controlling Nanomagnetic Particle Parameters. , 2019, , .		2
23	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
24	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
25	Ultrafast Electric Field Pulse Control of Giant Temperature Change in Ferroelectrics. Physical Review Letters, 2018, 120, 055901.	2.9	21
26	Combining inverse and conventional pyroelectricity in antiferroelectric thin films for energy conversion. Journal of Materials Chemistry C, 2018, 6, 9828-9834.	2.7	12
27	Resonant domain-wall-enhanced tunable microwave ferroelectrics. Nature, 2018, 560, 622-627.	13.7	82
28	Comment on â€œUltrafast terahertz-field-driven ionic response in ferroelectric BaTiO3 â€• Physical Review B, 2018, 97, .	1.1	0
29	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></mml:math> ' â€• Physical Review B, 2018, 97, .	1.1	1
30	Giant Bulk Photovoltaic Effect in Vinylene-Linked Hybrid Heterocyclic Polymer. Journal of Physical Chemistry C, 2017, 121, 6500-6507.	1.5	15
31	Large polarization gradients and temperature-stable responses in compositionally-graded ferroelectrics. Nature Communications, 2017, 8, 14961.	5.8	60
32	Asymmetry in mechanical polarization switching. Applied Physics Letters, 2017, 110, .	1.5	20
33	Slush-like polar structures in single-crystal relaxors. Nature, 2017, 546, 391-395.	13.7	201
34	Origin of stationary domain wall enhanced ferroelectric susceptibility. Physical Review B, 2017, 95, .	1.1	15
35	Light-induced picosecond rotational disordering of the inorganic sublattice in hybrid perovskites. Science Advances, 2017, 3, e1602388.	4.7	149
36	Multiscale simulations of defect dipoleâ€“enhanced electromechanical coupling at dilute defect concentrations. Applied Physics Letters, 2017, 111, .	1.5	17

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37	Origin of Negative Longitudinal Piezoelectric Effect. Physical Review Letters, 2017, 119, 207601.	2.9	63
38	Stable charged antiparallel domain walls in hyperferroelectrics. Journal of Physics Condensed Matter, 2017, 29, 244003.	0.7	10
39	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
40	Shift current bulk photovoltaic effect in polar materialsâ€”hybrid and oxide perovskites and beyond. Npj Computational Materials, 2016, 2, .	3.5	246
41	High Chloride Doping Levels Stabilize the Perovskite Phase of Cesium Lead Iodide. Nano Letters, 2016, 16, 3563-3570.	4.5	247
42	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
43	Electron-beam-induced ferroelectric domain behavior in the transmission electron microscope: Toward deterministic domain patterning. Physical Review B, 2016, 94, .	1.1	26
44	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></m Physical Review B, 2016, 94, .	1.1	52
45	Intrinsic ferroelectric switching from first principles. Nature, 2016, 534, 360-363.	13.7	151
46	Strain-Induced Ferroelectric Topological Insulator. Nano Letters, 2016, 16, 1663-1668.	4.5	82
47	Photoferroelectric and Photopiezoelectric Properties of Organometal Halide Perovskites. Journal of Physical Chemistry Letters, 2016, 7, 1460-1465.	2.1	73
48	Asymmetric Response of Ferroelastic Domain-Wall Motion under Applied Bias. ACS Applied Materials & Interfaces, 2016, 8, 2935-2941.	4.0	11
49	Toward Deterministic Switching in Ferroelectric Systems: Insight Gained from In Situ TEM. Microscopy and Microanalysis, 2015, 21, 1347-1348.	0.2	0
50	Ultrafast Terahertz Gating of the Polarization and Giant Nonlinear Optical Response in BiFeO₃ Thin Films. Advanced Materials, 2015, 27, 6371-6375.	11.1	47
51	Theoretical Study of Intermolecular Chain Transfer to Polymer Reactions of Alkyl Acrylates. Industrial & Engineering Chemistry Research, 2015, 54, 4148-4165.	1.8	20
52	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
53	Quantum pressure and chemical bonding: Influence of magnetic fields on electron localization. Physical Review B, 2015, 92, .	1.1	8
54	Polarization Dependence of Water Adsorption to CH₃NH₃PbI₃ (001) Surfaces. Journal of Physical Chemistry Letters, 2015, 6, 4371-4378.	2.1	111

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55	Rashba Spinâ€“Orbit Coupling Enhanced Carrier Lifetime in CH₃NH₃PbI₃. Nano Letters, 2015, 15, 7794-7800.	4.5	438
56	Material Innovation in Advancing Organometal Halide Perovskite Functionality. Journal of Physical Chemistry Letters, 2015, 6, 4862-4872.	2.1	37
57	Ferroelectric polarization reversal via successive ferroelastic transitions. Nature Materials, 2015, 14, 79-86.	13.3	216
58	Backbiting and Î²-scission reactions in free-radical polymerization of methyl acrylate. International Journal of Quantum Chemistry, 2014, 114, 345-360.	1.0	38
59	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
60	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
61	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
62	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
63	Exploration of the intrinsic inertial response of ferroelectric domain walls via molecular dynamics simulations. Applied Physics Letters, 2013, 103, .	1.5	13
64	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
65	Effect of Microphase Separation on the Protein Resistance of a Polymeric Surface. Langmuir, 2009, 25, 9467-9472.	1.6	40