

# Jibao Lu

## List of Publications by Year in descending order

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49  
papers

3,151  
citations

279798

23  
h-index

302126

39  
g-index

50  
all docs

50  
docs citations

50  
times ranked

4779  
citing authors

#	ARTICLE	IF	CITATIONS
1	Electronic and magnetic properties of perfect, vacancy-doped, and nonmetal adsorbed MoSe <sub>2</sub> , MoTe <sub>2</sub> and WS <sub>2</sub> monolayers. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 15546.	2.8	428
2	Modeling Molecular Interactions in Water: From Pairwise to Many-Body Potential Energy Functions. <i>Chemical Reviews</i> , 2016, 116, 7501-7528.	47.7	314
3	Hydrogenated titania: synergy of surface modification and morphology improvement for enhanced photocatalytic activity. <i>Chemical Communications</i> , 2012, 48, 5733.	4.1	285
4	Synergistic effect of crystal and electronic structures on the visible-light-driven photocatalytic performances of Bi <sub>2</sub> O <sub>3</sub> polymorphs. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 15468.	2.8	261
5	Composition Dependence of the Photocatalytic Activities of BiOCl <sub>1-x</sub> Br <sub>x</sub> Solid Solutions under Visible Light. <i>Chemistry - A European Journal</i> , 2011, 17, 9342-9349.	3.3	196
6	Ultrahigh-Aspect-Ratio Boron Nitride Nanosheets Leading to Superhigh In-Plane Thermal Conductivity of Foldable Heat Spreader. <i>ACS Nano</i> , 2021, 15, 6489-6498.	14.6	191
7	Hierarchical TiO <sub>2</sub> Microspheres: Synergetic Effect of {001} and {101} Facets for Enhanced Photocatalytic Activity. <i>Chemistry - A European Journal</i> , 2011, 17, 15032-15038.	3.3	180
8	A Paper-Like Inorganic Thermal Interface Material Composed of Hierarchically Structured Graphene/Silicon Carbide Nanorods. <i>ACS Nano</i> , 2019, 13, 1547-1554.	14.6	131
9	Enhanced thermal conductivity for Ag-deposited alumina sphere/epoxy resin composites through manipulating interfacial thermal resistance. <i>Composites Part A: Applied Science and Manufacturing</i> , 2018, 107, 561-569.	7.6	115
10	Coarse-Graining of TIP4P/2005, TIP4P-Ew, SPC/E, and TIP3P to Monatomic Anisotropic Water Models Using Relative Entropy Minimization. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4104-4120.	5.3	108
11	Suppressing Photoinduced Charge Recombination via the Lorentz Force in a Photocatalytic System. <i>Advanced Science</i> , 2019, 6, 1901244.	11.2	101
12	Improving thermal conductivity of polymer composites by reducing interfacial thermal resistance between boron nitride nanotubes. <i>Composites Science and Technology</i> , 2018, 165, 322-330.	7.8	98
13	Soft and Self-Adhesive Thermal Interface Materials Based on Vertically Aligned, Covalently Bonded Graphene Nanowalls for Efficient Microelectronic Cooling. <i>Advanced Functional Materials</i> , 2021, 31, 2104062.	14.9	95
14	Effective increasing of optical absorption and energy conversion efficiency of anatase TiO <sub>2</sub> nanocrystals by hydrogenation. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 18063.	2.8	92
15	Chemical and optical properties of carbon-doped TiO <sub>2</sub> : A density-functional study. <i>Applied Physics Letters</i> , 2012, 100, 102114.	3.3	54
16	Effect of chemical functionalization on the thermal conductivity of 2D hexagonal boron nitride. <i>Applied Physics Letters</i> , 2018, 113, .	3.3	43
17	N- and Mo-doping Bi <sub>2</sub> WO <sub>6</sub> in photocatalytic water splitting. <i>Computational Materials Science</i> , 2013, 67, 88-92.	3.0	39
18	Effect of Polymer Architecture on the Nanophase Segregation, Ionic Conductivity, and Electro-Osmotic Drag of Anion Exchange Membranes. <i>Journal of Physical Chemistry C</i> , 2019, 123, 8717-8726.	3.1	35

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19	Relationship between the line of density anomaly and the lines of melting, crystallization, cavitation, and liquid spinodal in coarse-grained water models. <i>Journal of Chemical Physics</i> , 2016, 144, 234507.	3.0	32
20	Tuning of the Surface-Exposing and Photocatalytic Activity for AgX (X = Cl and Br): A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 19372-19378.	3.1	31
21	High-Resolution Coarse-Grained Model of Hydrated Anion-Exchange Membranes that Accounts for Hydrophobic and Ionic Interactions through Short-Ranged Potentials. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 245-264.	5.3	31
22	Facile and Efficient Welding of Silver Nanowires Based on UVA-Induced Nanoscale Photothermal Process for Roll-to-Roll Manufacturing of High-Performance Transparent Conducting Films. <i>Advanced Materials Interfaces</i> , 2019, 6, 1801635.	3.7	30
23	Multiscale Modeling of Structure, Transport and Reactivity in Alkaline Fuel Cell Membranes: Combined Coarse-Grained, Atomistic and Reactive Molecular Dynamics Simulations. <i>Polymers</i> , 2018, 10, 1289.	4.5	26
24	First-principles study of the electronic and magnetic properties of oxygen-deficient rutile TiO <sub>2</sub> (110) surface. <i>Journal of Solid State Chemistry</i> , 2011, 184, 1148-1152.	2.9	23
25	A comprehensive study of pyrazine-contained and low-temperature curable polyimide. <i>Polymer</i> , 2021, 228, 123963.	3.8	23
26	Effect of Electronegativity and Charge Balance on the Visible-Light-Responsive Photocatalytic Activity of Nonmetal Doped Anatase TiO <sub>2</sub> . <i>International Journal of Photoenergy</i> , 2012, 2012, 1-8.	2.5	22
27	Density Functional Characterization of Pure and Alkaline Earth Metal-Doped Bi <sub>12</sub> GeO <sub>20</sub> , Bi <sub>12</sub> SiO <sub>20</sub> , and Bi <sub>12</sub> TiO <sub>20</sub> Photocatalysts. <i>ChemCatChem</i> , 2011, 3, 378-385.	3.7	21
28	Structure and Electronic Properties and Phase Stabilities of the Cd <sub>1-x</sub> Zn <sub>x</sub> S Solid Solution in the Range of 0 ≤ x ≤ 1. <i>ChemPhysChem</i> , 2012, 13, 147-154.	2.1	21
29	Synergistic effects of codopants on photocatalytic O <sub>2</sub> evolution in BiVO <sub>4</sub> . <i>Solid State Sciences</i> , 2013, 24, 79-84.	3.2	20
30	Parameterization of a coarse-grained model with short-ranged interactions for modeling fuel cell membranes with controlled water uptake. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17698-17707.	2.8	20
31	3D interconnected high aspect ratio tellurium nanowires in epoxy nanocomposites: serving as thermal conductive expressway. <i>Journal of Applied Polymer Science</i> , 2019, 136, 47054.	2.6	17
32	Numerical homogenization of thermal conductivity of particle-filled thermal interface material by fast Fourier transform method. <i>Nanotechnology</i> , 2021, 32, 265708.	2.6	13
33	Mechanism of Facilitation of Ion Mobility in Low-Water-Content Fuel Cell Membranes. <i>Journal of Physical Chemistry C</i> , 2021, 125, 27703-27713.	3.1	12
34	Width and Clustering of Ion-Conducting Channels in Fuel Cell Membranes Are Insensitive to the Length of Ion Tethers. <i>Journal of Physical Chemistry C</i> , 2021, 125, 27693-27702.	3.1	11
35	Topological phase transition and unexpected mass acquisition of Dirac fermion in TlBi(S <sub>1-x</sub> Se <sub>x</sub> ) <sub>2</sub> . <i>Applied Physics Letters</i> , 2012, 101, 182101.	3.3	6
36	Characterization and Verification of Viscoelastic Constitutive Parameters of Underfill Material. , 2021, , .		5

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37	Effect of hydrogen bonds on the thermal transport in a precisely branched polyethylene with ordered and amorphous structures. Computational Materials Science, 2022, 205, 111191.	3.0	5
38	Comparative Analysis of Temperature-induced Micro-scale Deformation of Package by Experiment and Finite Element Analysis. , 2021, , .		3
39	Viscoelastic Characterization and Simulation of Thermal Interface Materials. , 2021, , .		3
40	Study of the interfacial adhesion properties of a novel Self-healable siloxane polymer material via molecular dynamics simulation. Applied Surface Science, 2022, 583, 152471.	6.1	3
41	Mold Flow Simulation Analysis of Molded Underfill in an Ultra-thin High-Density Package. , 2022, , .		3
42	The Synthetic Effects of Iron with Sulfur and Fluorine on Photoabsorption and Photocatalytic Performance in Codoped. International Journal of Photoenergy, 2012, 2012, 1-7.	2.5	2
43	The Effect of Thermal-Induced Warpage and Degeneration of Thermal Interface Materials on the Thermal Performance of a Flip-Chip Package. , 2021, , .		1
44	Role of water environment in chemical degradation of a covalent organic framework tethered with quaternary ammonium for anion exchange membranes. RSC Advances, 2022, 12, 19240-19245.	3.6	1
45	Comparison between two numerical methods for the computation of thermal conductivities of particulate composites: FEM and GeoDict. , 2021, , .		0
46	Numerical analysis of the microscopic factors influencing the thermal conductivity of Al <sub>2</sub> O <sub>3</sub> / AlN polymer composites. , 2021, , .		0
47	Orthogonal Experiment for Analyzing the Impact of Thermal Stress on the Reliability of an EMC Package. , 2021, , .		0
48	Numerical analysis on the effect of microstructures on the thermal and mechanical properties of carbon fiber / Al <sub>2</sub> O <sub>3</sub> thermal pad. , 2021, , .		0
49	The Influence of Properties of Solder Joint on the Stress of Underfill in Flip Chip Package. , 2022, , .		0