

# Lijie Li

## List of Publications by Year in descending order

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68  
papers

1,032  
citations

430874  
18  
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501196  
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69  
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69  
docs citations

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times ranked

749  
citing authors

#	ARTICLE	IF	CITATIONS
1	Polymer-based lightweight materials for electromagnetic interference shielding: a review. <i>Journal of Materials Science</i> , 2021, 56, 6549-6580.	3.7	93
2	Preparation, characterization and thermal risk evaluation of dihydroxylammonium 5, 5- $\epsilon^2$ -bistetrazole-1, 1- $\epsilon^2$ -diolate based polymer bonded explosive. <i>Journal of Hazardous Materials</i> , 2017, 338, 208-217.	12.4	56
3	Effects of Additives on $\epsilon^2$ -HNIW Crystal Morphology and Impact Sensitivity. <i>Propellants, Explosives, Pyrotechnics</i> , 2012, 37, 77-82.	1.6	52
4	Thermal decomposition mechanism study of 3-nitro-1,2,4-triazol-5-one (NTO): Combined TG-FTIR-MS techniques and ReaxFF reactive molecular dynamics simulations. <i>Fuel</i> , 2021, 295, 120655.	6.4	44
5	Thermolysis, nonisothermal decomposition kinetics, calculated detonation velocity and safety assessment of dihydroxylammonium 5, 5- $\epsilon^2$ -bistetrazole-1, 1- $\epsilon^2$ -diolate. <i>Journal of Thermal Analysis and Calorimetry</i> , 2016, 126, 473-480.	3.6	43
6	Morphology control of 3-nitro-1,2,4-triazole-5-one (NTO) by molecular dynamics simulation. <i>CrystEngComm</i> , 2018, 20, 6252-6260.	2.6	35
7	Surface Modification for Improving the Photocatalytic Polymerization of 3,4-Ethylenedioxythiophene over Inorganic Lead Halide Perovskite Quantum Dots. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 451-460.	8.0	34
8	Bridged Ti <sub>3</sub> C <sub>2</sub> T <sub>X</sub> MXene Film with Superior Oxidation Resistance and Structural Stability for High-Performance Flexible Supercapacitors. <i>ACS Applied Energy Materials</i> , 2022, 5, 2898-2908.	5.1	34
9	Molecular dynamic simulations on TKX-50/HMX cocrystal. <i>RSC Advances</i> , 2017, 7, 6795-6799.	3.6	30
10	Polytetrafluoroethylene-assisted N/F co-doped hierarchically porous carbon as a high performance electrode for supercapacitors. <i>Journal of Colloid and Interface Science</i> , 2019, 545, 25-34.	9.4	30
11	Thermal hazard assessment of 4,10-dinitro-2,6,8,12-tetraoxa-4,10-diazaisowutrzitane (TEX) by accelerating rate calorimeter (ARC). <i>Journal of Thermal Analysis and Calorimetry</i> , 2016, 126, 467-471.	3.6	28
12	Nitrogen-rich 4,4- $\epsilon^2$ -azo bis(1,2,4-triazolone) salts—the synthesis and promising properties of a new family of high-density insensitive materials. <i>Dalton Transactions</i> , 2016, 45, 3590-3598.	3.3	27
13	Prediction of crystal morphology of 3,4-Dinitro-1H-pyrazole (DNP) in different solvents. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 75, 62-70.	2.4	24
14	Reactive molecular dynamics simulations on the thermal decompositions and oxidations of TKX-50 and twinned TKX-50. <i>CrystEngComm</i> , 2020, 22, 2593-2600.	2.6	24
15	The crossover behavior of bromine species in the metal-free flow battery. <i>Journal of Applied Electrochemistry</i> , 2017, 47, 261-272.	2.9	23
16	First-principles calculation of quantum capacitance of metals doped graphenes and nitrogen/metals co-doped graphenes: designing strategies for supercapacitor electrodes. <i>Journal of Materials Science</i> , 2019, 54, 483-492.	3.7	23
17	The effect of solution conditions on the crystal morphology of $\epsilon^2$ -HMX by molecular dynamics simulations. <i>Journal of Crystal Growth</i> , 2019, 507, 38-45.	1.5	22
18	Quantitative Determination of $\epsilon^2$ -phase in polymorphic HNIW using X-ray Diffraction Patterns. <i>Propellants, Explosives, Pyrotechnics</i> , 2008, 33, 467-471.	1.6	20

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19	The study of external growth environments on the crystal morphology of $\mu$ -HNIW by molecular dynamics simulation. <i>Journal of Materials Science</i> , 2018, 53, 12921-12936.	3.7	20
20	Preparation and Characterization of Cyclotrimethylenetrinitramine (RDX) with Reduced Sensitivity. <i>Materials</i> , 2017, 10, 974.	2.9	19
21	The Critical Role of Oxygen-Containing Functional Groups in the Etching Behavior of Activators to Carbon Materials. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 1646-1655.	6.7	19
22	A simple ratiometric and colorimetric chemosensor for the selective detection of fluoride in DMSO buffered solution. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 153, 194-198.	3.9	18
23	Study on a novel high energetic and insensitive munitions formulation: TKX-50 based melt cast high explosive. <i>RSC Advances</i> , 2017, 7, 31485-31492.	3.6	18
24	Molecular dynamics simulations on miscibility, glass transition temperature and mechanical properties of PMMA/DBP binary system. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 84, 182-188.	2.4	17
25	Preparation and performances characterization of HNIW/NTO-based high-energetic low vulnerable polymer-bonded explosive. <i>Journal of Thermal Analysis and Calorimetry</i> , 2020, 139, 3589-3602.	3.6	17
26	Preparation, nonisothermal decomposition kinetics, heat capacity, and safety parameters of TKX-50-based PBX. <i>Journal of Thermal Analysis and Calorimetry</i> , 2018, 131, 3193-3199.	3.6	16
27	Study on Cellulose Acetate Butyrate/Plasticizer Systems by Molecular Dynamics Simulation and Experimental Characterization. <i>Polymers</i> , 2020, 12, 1272.	4.5	16
28	Squaramide-based lab-on-a-molecule for the detection of silver ion and nitroaromatic explosives. <i>RSC Advances</i> , 2015, 5, 96665-96669.	3.6	15
29	Effects of the N/S codoping configuration and ternary doping on the quantum capacitance of graphene. <i>Journal of Materials Science</i> , 2019, 54, 8995-9003.	3.7	14
30	Dissolution Properties of Dihydroxylammonium 5,5'-Bistetrazole-1,1'-diolate and Disodium 5,5'-Bistetrazole-1,1'-diolate in Water. <i>Journal of Energetic Materials</i> , 2016, 34, 416-425.	2.0	12
31	Thermal behavior and thermo-kinetic studies of 5,5'-bistetrazole-1,1'-diolate (1,1-BTO). <i>Journal of Thermal Analysis and Calorimetry</i> , 2017, 129, 1265-1270.	3.6	12
32	Preparation and thermal properties study of HNIW/FOX-7 based high energy polymer bonded explosive (PBX) with low vulnerability to thermal stimulations. <i>Journal of Energetic Materials</i> , 2020, 38, 83-97.	2.0	12
33	Preparation, Crystal Structure and Properties of a New Crystal Form of Diammonium 5,5'-bistetrazole-1,1'-diolate. <i>Chinese Journal of Chemistry</i> , 2015, 33, 1229-1234.	4.9	11
34	The novel compound dimethylamine-5,5'-bistetrazole-1,1'-diolate: crystal structure, thermal investigation, safety evaluation and theoretical studies. <i>RSC Advances</i> , 2017, 7, 18523-18528.	3.6	10
35	Density Functional Theory (DFT) Study on the Structures and Energetic Properties of Isomers of Tetranitro-bis-1,2,4-triazoles. <i>ACS Omega</i> , 2020, 5, 19464-19468.	3.5	10
36	Theoretical study of the heats of formation, detonation properties, and bond dissociation energies of substituted bis-1,2,4-triazole compounds. <i>Journal of Molecular Modeling</i> , 2018, 24, 85.	1.8	9

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37	Heat effects of NTO synthesis in nitric acid solution. Journal of Thermal Analysis and Calorimetry, 2017, 128, 301-310.	3.6	8
38	Molecular dynamics investigation on the morphology of HNIW affected by the growth condition. Journal of Energetic Materials, 2019, 37, 44-56.	2.0	8
39	Reactive molecular dynamics simulation of thermal decomposition for nano-FOX-7. Applied Physics A: Materials Science and Processing, 2021, 127, 1.	2.3	8
40	Ameliorating the performances of 3,4-bis(4-nitrofurazano-3-yl)furoxan (DNTF) by establishing tannic acid (TA) interface layer on DNTF surface. Chemical Engineering Journal, 2022, 434, 134513.	12.7	8
41	Molecular dynamic simulations for FOX-7 and FOX-7 based PBXs. Journal of Molecular Modeling, 2018, 24, 145.	1.8	7
42	Thermal decomposition and thermal stability of potassium 3,3-dinitrimino-5,5-bis(1H-1,2,4-triazole). Journal of Thermal Analysis and Calorimetry, 2018, 133, 1563-1569.	3.6	6
43	Measurement and Correlation of Solubilities of 5,5-Dinitramino-3,3-bis[1,2,4-triazolate] Carbohydrazide Salt (CBNT) in Various Pure Solvents and a Binary Mixture (Dimethyl Sulfoxide + Water) from 298.15 to 343.15 K. Journal of Chemical & Engineering Data, 2019, 64, 3874-3881.	1.9	6
44	Investigation into the Temperature Adaptability of HNIW-based PBXs. Propellants, Explosives, Pyrotechnics, 2019, 44, 327-336.	1.6	6
45	Thermal safety assessment and thermo-kinetic parameters of 5,5-dinitramino-3,3-bis[1,2,4-triazolate] carbohydrazide salt (CBNT). Journal of Thermal Analysis and Calorimetry, 2021, 144, 647-655.	3.6	6
46	Rational Construction of Cobalt Sulfide Nanoparticles Embedded in Hollow N, P, S Codoped Carbon Shells for Enhanced Supercapacitor Performance. ACS Applied Energy Materials, 2022, 5, 1436-1446.	5.1	6
47	Dissolution thermodynamics of dihydroxylammonium 5,5-bistetrazole-1,1-diolate in water at $T = (298.15, 313.15, 323.15, 333.15, 343.15, 353.15, 363.15, 373.15, 383.15, 393.15, 403.15, 413.15, 423.15, 433.15, 443.15, 453.15, 463.15, 473.15, 483.15, 493.15, 503.15, 513.15, 523.15, 533.15, 543.15, 553.15, 563.15, 573.15, 583.15, 593.15, 603.15, 613.15, 623.15, 633.15, 643.15, 653.15, 663.15, 673.15, 683.15, 693.15, 703.15, 713.15, 723.15, 733.15, 743.15, 753.15, 763.15, 773.15, 783.15, 793.15, 803.15, 813.15, 823.15, 833.15, 843.15, 853.15, 863.15, 873.15, 883.15, 893.15, 903.15, 913.15, 923.15, 933.15, 943.15, 953.15, 963.15, 973.15, 983.15, 993.15) K. Journal of Chemical & Engineering Data, 2021, 66, 3897-3910.$	3.6	5
48	A molecular dynamics study and detonation parameters calculation of 5,5-dinitramino-3,3-bis[1,2,4-triazolate] carbohydrazide salt (CBNT) and its PBXs. Journal of Energetic Materials, 2020, 38, 283-294.	2.0	5
49	Solubilities of 2,6-Diamino-3,5-dinitropyrazine-1-oxide in the Binary Mixtures of DMSO+H <sub>2</sub> O, DMF+H <sub>2</sub> O and NMP+H <sub>2</sub> O in the Temperature Range from 293.15 to 323.15 K under the Atmospheric Pressure. Propellants, Explosives, Pyrotechnics, 2020, 45, 503-508.	1.6	5
50	Measurement and Correlation of Solubilities of 3-Nitro-1,2,4-triazol-5-one (NTO) in 10 Pure Solvents and 3 Binary Solvents from 278.15 to 328.15 K. Journal of Chemical & Engineering Data, 2021, 66, 3897-3910.	1.9	5
51	Empirical Kinetics Equation of the Synthesis of NTO in Nitric Acid. Propellants, Explosives, Pyrotechnics, 2016, 41, 1085-1091.	1.6	4
52	Preparation, crystal structure, thermal behavior, and theoretical studies of N,N-dinitro-4,4-azo-bis(1,2,4-triazolone) (DNZTO). Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2016, 71, 197-204.	0.7	4
53	Theoretical study on the weak interaction and energy performance of nitroformate salts and nitroformate-based propellant formulations. Journal of Molecular Modeling, 2019, 25, 285.	1.8	4
54	Morphology prediction of dihydroxylammonium 5,5-bistetrazole-1,1-diolate (TKX-50) crystal in different solvent systems using modified attachment energy model. Chinese Journal of Chemical Engineering, 2023, 53, 181-193.	3.5	4

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55	Synthesis and Characterization of 1,5-dinitro-2,6-bis(trinitromethyl)-3a,4a,7a,8a-tetrahydro-1,4-dioxino[2,3-d:5,6-d']diimidazole (DMTNDI). Propellants, Explosives, Pyrotechnics, 2013, 38, 658-664.	3.3	3
56	Crystal structure of 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazatetracyclo[5.5.0.0.5.9.0.3.11]dodecane 1/3 hydrate, C <sub>6</sub> H <sub>8</sub> N <sub>12</sub> O <sub>13</sub> . Zeitschrift Fur Kristallographie - New Crystal Structures, 2016, 231, 491-492.	0.3	3
57	Miscibility, Glass Transition Temperature and Mechanical Properties of NC/DBP Binary Systems by Molecular Dynamics. Propellants, Explosives, Pyrotechnics, 2018, 43, 559-567.	1.6	3
58	The crystal structure and thermal analysis of ZTO and its solvent adducts. Research on Chemical Intermediates, 2016, 42, 4333-4340.	2.7	2
59	Dissolution properties of 5,5'-bistetrazole-1, 1'-dihydroxy and disodium 5,5'-bistetrazole-1, 1'-diolate in dimethyl sulfoxide. Journal of Thermal Analysis and Calorimetry, 2017, 128, 615-620.	3.6	2
60	Shock Initiation Investigation of a Pressed Trinitrotoluene Explosive. Propellants, Explosives, Pyrotechnics, 2021, 46, 1717.	1.6	2
61	Investigation of the effect of the CAB/A3 system on HNIW-based PBXs using molecular dynamics. Journal of Molecular Modeling, 2018, 24, 186.	1.8	1
62	Organic-Inorganic Artificial Ion Channel Polyvinylidene Fluoride Membranes for Controllable Selectivity Transport of Alkali Metal Cations. Membranes, 2020, 10, 174.	3.0	1
63	Design and properties of N,N'-linked bis-1,2,4-triazoles compounds as promising energetic materials. Journal of Molecular Modeling, 2020, 26, 130.	1.8	1
64	A novel ternary energetic compound: DAF/DNP/H <sub>2</sub> O cocrystal. Journal of Energetic Materials, 0, , 1-13.	2.0	1
65	The effect of solvents on the morphology of NTO crystal by molecular dynamics. Journal of Physics: Conference Series, 2022, 2285, 012034.	0.4	1
66	Crystal structure of hexaaquamagnesium(II) 5,5'-bitetrazole-1,1'-diolate, C <sub>2</sub> H <sub>12</sub> N <sub>8</sub> O <sub>8</sub> Mg. Zeitschrift Fur Kristallographie - New Crystal Structures, 2016, 231, 305-306.	0.3	0
67	Crystal structure of tetraqua((E)-4,4'-((diazene-1,2-diyl)bis(5-oxo-4,5-dihydro-1,2,4-triazol-1-ylidene)-N <sub>2</sub> O)barium(II), C <sub>4</sub> H <sub>10</sub> N <sub>8</sub> O <sub>6</sub> Ba. Zeitschrift Fur Kristallographie - New Crystal Structures, 2016, 231, 503-504.	0.3	0
68	The influence of temperature environmental on performance of HNIW/FOX-7 based PBXs. Scientific Reports, 2022, 12, 4988.	3.3	0