

James P Lewis

List of Publications by Year in descending order

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71
papers

6,743
citations

109264

35
h-index

88593

70
g-index

71
all docs

71
docs citations

71
times ranked

9602
citing authors

#	ARTICLE	IF	CITATIONS
1	A Database and Evaluation Methodology for Optical Flow. International Journal of Computer Vision, 2011, 92, 1-31.	10.9	1,565
2	Origin of Photocatalytic Activity of Nitrogen-Doped TiO ₂ Nanobelts. Journal of the American Chemical Society, 2009, 131, 12290-12297.	6.6	1,112
3	Shape-Enhanced Photocatalytic Activity of Single-Crystalline Anatase TiO ₂ (101) Nanobelts. Journal of the American Chemical Society, 2010, 132, 6679-6685.	6.6	680
4	Product Selectivity Controlled by Zeolite Crystals in Biomass Hydrogenation over a Palladium Catalyst. Journal of the American Chemical Society, 2016, 138, 7880-7883.	6.6	262
5	Advances and applications in the Fermi-IREBALL <i>ab initio</i> tight-binding molecular dynamics formalism. Physica Status Solidi (B): Basic Research, 2011, 248, 1989-2007.	0.7	207
6	Artificial intelligence: A powerful paradigm for scientific research. Innovation(China), 2021, 2, 100179.	5.2	200
7	Properties of amorphous and crystalline titanium dioxide from first principles. Journal of Materials Science, 2012, 47, 7515-7521.	1.7	173
8	Effects of dopant states on photoactivity in carbon-doped TiO ₂ . Journal of Physics Condensed Matter, 2005, 17, L209-L213.	0.7	145
9	Visible light plasmonic heating of Au-ZnO for the catalytic reduction of CO ₂ . Nanoscale, 2013, 5, 6968.	2.8	139
10	Selective Catalytic Production of 5-Hydroxymethylfurfural from Glucose by Adjusting Catalyst Wettability. ChemSusChem, 2014, 7, 402-406.	3.6	119
11	Dynamically Amorphous Character of Electronic States in Poly(dA)-Poly(dT) DNA. Journal of Physical Chemistry B, 2003, 107, 2581-2587.	1.2	106
12	Machine-Learning Prediction of CO Adsorption in Thiolated, Ag-Alloyed Au Nanoclusters. Journal of the American Chemical Society, 2018, 140, 17508-17514.	6.6	104
13	Synthesis, Characterization, Electronic Structure, and Photocatalytic Behavior of CuGaO ₂ and CuGa _{1-x} Fe _x O ₂ ($x = 0.25, 0.5, 0.75, 1$). Journal of Physical Chemistry C, 2011, 115, 104314-104324.	1.1	78
14	First-principles calculations for nitrogen-containing single-walled carbon nanotubes. Journal of Applied Physics, 2003, 94, 2398-2402.	1.1	93
15	Ab Initio Calculations of Reactive Pathways for $\hat{1}\pm$ -Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine ($\hat{1}\pm$ -HMX). Journal of Physical Chemistry A, 2000, 104, 11384-11389.	1.1	82
16	Batrachochytrium salamandrivorans: The North American Response and a Call for Action. PLoS Pathogens, 2015, 11, e1005251.	2.1	82
17	Activity and Selectivity in Nitroarene Hydrogenation over Au Nanoparticles on the Edge/Corner of Anatase. ACS Catalysis, 2016, 6, 4110-4116.	5.5	79
18	Visible light photocatalytic activity in nitrogen-doped TiO ₂ nanobelts. Applied Physics Letters, 2009, 94, 093101.	1.5	78

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19	Intermolecular Cross-Double-Michael Addition between Nitro and Carbonyl Activated Olefins as a New Approach in C-C Bond Formation. <i>Organic Letters</i> , 2007, 9, 4495-4498.	2.4	75
20	Electronic-structure-based molecular-dynamics method for large biological systems: Application to the 10 basepair poly(dG)·poly(dC) DNA double helix. <i>Physical Review B</i> , 1997, 55, 6880-6887.	1.1	69
21	Superior catalytic properties in aerobic oxidation of olefins over Au nanoparticles on pyrrolidone-modified SBA-15. <i>Journal of Catalysis</i> , 2011, 281, 30-39.	3.1	65
22	Theoretical Investigation of the Cyclic Peptide System Cyclo[(d-Ala-Glu-d-Ala-Gln) _{m=1-4}]. <i>Journal of Physical Chemistry B</i> , 1997, 101, 10576-10583.	1.2	61
23	Nonadiabatic Ensemble Simulations of <i>cis</i> -Stilbene and <i>cis</i> -Azobenzene Photoisomerization. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 14-23.	2.3	58
24	Electronic Structure Calculation of the Structures and Energies of the Three Pure Polymorphic Forms of Crystalline HMX. <i>Journal of Physical Chemistry B</i> , 2000, 104, 1009-1013.	1.2	52
25	The application of approximate density functionals to complex systems. <i>International Journal of Quantum Chemistry</i> , 1998, 69, 327-340.	1.0	46
26	Linear-scaling quantum mechanical calculations of biological molecules: The divide-and-conquer approach. <i>Computational Materials Science</i> , 1998, 12, 259-277.	1.4	45
27	Synthesis, characterization, and photocatalytic activity of Au-ZnO nanopyramids. <i>Journal of Materials Chemistry A</i> , 2015, 3, 15141-15147.	5.2	45
28	Aerobic homocoupling of phenylboronic acid on Mg-Al mixed-oxides-supported Au nanoparticles. <i>Journal of Catalysis</i> , 2013, 298, 186-197.	3.1	44
29	Controlling Ag-doping in [Ag _x Au _{25-x} (SC ₆ H ₁₁) ₁₈] ⁺ nanoclusters: cryogenic optical, electronic and electrocatalytic properties. <i>Nanoscale</i> , 2017, 9, 19183-19190.	1.8	43
30	Rationally Designed Metal Cocatalyst for Selective Photosynthesis of Bibenzyls via Dehalogenative C-C Homocoupling. <i>ACS Catalysis</i> , 2021, 11, 4338-4348.	5.5	43
31	Cysteine Interaction with Au ₅₅ Nanoparticle. <i>Journal of Physical Chemistry C</i> , 2012, 116, 25816-25823.	1.5	42
32	fireball/amber: An Efficient Local-Orbital DFT QM/MM Method for Biomolecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2185-2193.	2.3	42
33	Accelerated Discovery of Two-Dimensional Optoelectronic Octahedral Oxyhalides via High-Throughput <i>Ab Initio</i> Calculations and Machine Learning. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6734-6740.	2.1	40
34	A Machine-Driven Hunt for Global Reaction Coordinates of Azobenzene Photoisomerization. <i>Journal of the American Chemical Society</i> , 2018, 140, 285-290.	6.6	39
35	Active Species for the Ground-State Complex of Cytidine Deaminase: A Linear-Scaling Quantum Mechanical Investigation. <i>Journal of the American Chemical Society</i> , 1998, 120, 5407-5410.	6.6	38
36	Evaluation of functionalized isorecticular metal organic frameworks (IRMOFs) as smart nanoporous preconcentrators of RDX. <i>Sensors and Actuators B: Chemical</i> , 2010, 148, 459-468.	4.0	38

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37	First principles simulations of fluid water: The radial distribution functions. Journal of Chemical Physics, 1997, 106, 3696-3702.	1.2	36
38	Chemical Reactivity of Single-Walled Carbon Nanotubes to Amidogen from Density Functional Calculations. Journal of Physical Chemistry B, 2004, 108, 9599-9603.	1.2	35
39	Simplified electronic-structure model for hydrogen-bonded systems: Water. Physical Review B, 1994, 50, 10516-10530.	1.1	33
40	Energetics of intermolecular HONO formation in condensed-phase octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX). Chemical Physics Letters, 2003, 371, 588-593.	1.2	32
41	Design and Preparation of Supported Au Catalyst with Enhanced Catalytic Activities by Rationally Positioning Au Nanoparticles on Anatase. Journal of Physical Chemistry Letters, 2015, 6, 2345-2349.	2.1	32
42	BASE SEQUENCE EFFECTS ON CHARGE CARRIER GENERATION IN DNA: A THEORETICAL STUDY. International Journal of Modern Physics B, 2005, 19, 4331-4357.	1.0	28
43	Effect of Charge Distribution on RDX Adsorption in IRMOF-10. Langmuir, 2010, 26, 5942-5950.	1.6	27
44	Electronic Structures and Conductivity in Peptide Nanotubes. Journal of Physical Chemistry B, 2007, 111, 9093-9098.	1.2	23
45	A full quantum embedded cluster study of proton siting in chabazite. Chemical Physics Letters, 2001, 350, 128-134.	1.2	20
46	Interaction of the Explosive Molecules RDX and TATP with IRMOF-8. Journal of Physical Chemistry C, 2010, 114, 7535-7540.	1.5	20
47	Quantum Mechanics/Molecular Mechanics Free Energy Maps and Nonadiabatic Simulations for a Photochemical Reaction in DNA: Cyclobutane Thymine Dimer. Journal of Physical Chemistry Letters, 2016, 7, 4391-4397.	2.1	20
48	A Linear-Scaling Quantum Mechanical Investigation of Cytidine Deaminase. Journal of Computational Physics, 1999, 151, 242-263.	1.9	18
49	Hidden structure in amorphous solids. Physica Status Solidi (A) Applications and Materials Science, 2010, 207, 599-604.	0.8	18
50	Geometry and energetics of DNA basepairs and triplets from first principles quantum molecular relaxations. Biophysical Journal, 1995, 69, 1068-1076.	0.2	17
51	Calculation of non-adiabatic coupling vectors in a local-orbital basis set. Journal of Chemical Physics, 2013, 138, 154106.	1.2	17
52	Structural and catalytic properties of the Au ₂₅ Ag ₃ (SCH ₃) ₁₈ (x = 6, 7, 8) nanocluster. Physical Chemistry Chemical Physics, 2018, 20, 13747-13756.	1.3	17
53	Tripeptides on Gold Nanoparticles: Structural Differences between Two Reverse Sequences as Determined by Solid-State NMR and DFT Calculations. Journal of Physical Chemistry B, 2015, 119, 11998-12006.	1.2	16
54	Slow Relaxation of Surface Plasmon Excitations in Au ₅₅ : The Key to Efficient Plasmonic Heating in Au/TiO ₂ . Journal of Physical Chemistry Letters, 2016, 7, 1563-1569.	2.1	16

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55	Boosting Photocatalytic Hydrogen Production by Modulating Recombination Modes and Proton Adsorption Energy. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 5381-5386.	2.1	15
56	Effects of Vacancy and Ti Doping in 2D Janus MoSSe on Photocatalysis. <i>Journal of Physical Chemistry C</i> , 2021, 125, 11939-11949.	1.5	14
57	Electronic state and concentration of Fe ³⁺ in CuAl _{1-x} Fe _x O ₂ determined by magnetic measurements. <i>Journal of Magnetism and Magnetic Materials</i> , 2019, 471, 495-500.	1.0	12
58	Magnetic properties of Fe-doped CuAlO ₂ and role of impurities. <i>AIP Advances</i> , 2019, 9, .	0.6	12
59	Calculated photo-isomerization efficiencies of functionalized azobenzene derivatives in solar energy materials: azo-functional organic linkers for porous coordinated polymers. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 134208.	0.7	11
60	Localization of Frontier Orbitals on Anatase Nanoparticles Impacts Water Adsorption. <i>Journal of Physical Chemistry C</i> , 2009, 113, 16631-16637.	1.5	9
61	The reactive sites in faceted anatase nanoparticles. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 2037-2043.	0.7	9
62	Optical absorption and disorder in delafossites. <i>Applied Physics Letters</i> , 2017, 111, 012102.	1.5	8
63	Phonon Dynamics in Anisotropic Dilute CuAl _{1-x} Fe _x O ₂ Delafossite Alloys by a Weighted Dynamical Matrix Approach. <i>Journal of Physical Chemistry C</i> , 2019, 123, 30604-30612.	1.5	5
64	Differential electronic states observed during A ⁺ B DNA duplex conformational transitions. <i>Soft Matter</i> , 2009, 5, 685-690.	1.2	3
65	High-throughput evaluation in nitrogen doping of amorphous titanium dioxide. <i>Physica Status Solidi (B): Basic Research</i> , 2014, 251, 1225-1230.	0.7	3
66	Computational Insights into Morphology and Interface of Zeolite Catalysts: a Case Study of K-LTL Zeolite with Different Si/Al Ratios. <i>Journal of Physical Chemistry C</i> , 2018, 122, 24843-24850.	1.5	3
67	The structural information filtered features (SIFF) potential: Maximizing information stored in machine-learning descriptors for materials prediction. <i>Journal of Applied Physics</i> , 2020, 127, 215108.	1.1	3
68	Criteria for ductility in Cr alloys based on electronic structures. <i>Applied Physics Letters</i> , 2008, 93, 241903.	1.5	1
69	Failure of potassium dimer formation on the SiC(100)-(4 \times 4)-2 surface. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 2072-2075.	0.7	1
70	Tuning Surface Electron Spins on Fe ₃ O ₄ (111) through Chemisorption of Carbon Monoxide. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	1
71	Dual-Anion Vacancies in Apatite Systems. <i>ACS Applied Electronic Materials</i> , 2022, 4, 3655-3664.	2.0	0