

Sai Duan

List of Publications by Year in descending order

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66
papers

3,257
citations

257450

24
h-index

149698

56
g-index

68
all docs

68
docs citations

68
times ranked

5091
citing authors

#	ARTICLE	IF	CITATIONS
1	Atomically dispersed platinum supported on curved carbon supports for efficient electrocatalytic hydrogen evolution. <i>Nature Energy</i> , 2019, 4, 512-518.	39.5	756
2	Epitaxial Growth of Heterogeneous Metal Nanocrystals: From Gold Nano-octahedra to Palladium and Silver Nanocubes. <i>Journal of the American Chemical Society</i> , 2008, 130, 6949-6951.	13.7	719
3	Chemical Enhancement Effects in SERS Spectra: A Quantum Chemical Study of Pyridine Interacting with Copper, Silver, Gold and Platinum Metals. <i>Journal of Physical Chemistry C</i> , 2008, 112, 4195-4204.	3.1	207
4	Tailoring Au-core Pd-shell Pt-cluster nanoparticles for enhanced electrocatalytic activity. <i>Chemical Science</i> , 2011, 2, 531-539.	7.4	172
5	Core-Shell Nanostructure-Enhanced Raman Spectroscopy for Surface Catalysis. <i>Accounts of Chemical Research</i> , 2020, 53, 729-739.	15.6	136
6	Theoretical Modeling of Plasmon-Enhanced Raman Images of a Single Molecule with Subnanometer Resolution. <i>Journal of the American Chemical Society</i> , 2015, 137, 9515-9518.	13.7	92
7	SERS and DFT study of water on metal cathodes of silver, gold and platinum nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 2493.	2.8	73
8	The Realistic Domain Structure of As-Synthesized Graphene Oxide from Ultrafast Spectroscopy. <i>Journal of the American Chemical Society</i> , 2013, 135, 12468-12474.	13.7	64
9	Observation of inhomogeneous plasmonic field distribution in a nanocavity. <i>Nature Nanotechnology</i> , 2020, 15, 922-926.	31.5	62
10	Theoretical Study of Binding Interactions and Vibrational Raman Spectra of Water in Hydrogen-Bonded Anionic Complexes: $(\text{H}_2\text{O})_n^-$ ($n = 2$)	2.5	55
11	Mechanism for the Extremely Efficient Sensitization of Yb^{3+} Luminescence in CsPbCl_3 Nanocrystals. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 487-492.	4.6	55
12	Density functional theory study of surface-enhanced Raman scattering spectra of pyridine adsorbed on noble and transition metal surfaces. <i>Journal of Raman Spectroscopy</i> , 2005, 36, 533-540.	2.5	54
13	Visualization of Vibrational Modes in Real Space by Tip-Enhanced Non-Resonant Raman Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 1041-1045.	13.8	46
14	Beyond Mean-Field Microkinetics: Toward Accurate and Efficient Theoretical Modeling in Heterogeneous Catalysis. <i>ACS Catalysis</i> , 2018, 8, 5816-5826.	11.2	41
15	Real-time detection of single-molecule reaction by plasmon-enhanced spectroscopy. <i>Science Advances</i> , 2020, 6, eaba6012.	10.3	41
16	Selective Catalytic Dehydrogenative Oxidation of Bio-Polyols to Lactic Acid. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 13871-13878.	13.8	39
17	Roles of Plasmonic Excitation and Protonation on Photoreactions of <i>p</i> -Aminobenzenethiol on Ag Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2014, 118, 6893-6902.	3.1	33
18	Exceeding the volcano relationship in oxygen reduction/evolution reactions using single-atom-based catalysts with dual-active-sites. <i>Journal of Materials Chemistry A</i> , 2020, 8, 10193-10198.	10.3	33

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19	Microphotoelectrochemical Surface-Enhanced Raman Spectroscopy: Toward Bridging Hot-Electron Transfer with a Molecular Reaction. <i>Journal of the American Chemical Society</i> , 2020, 142, 8483-8489.	13.7	31
20	Effect of Intrinsic Properties of Metals on the Adsorption Behavior of Molecules: Benzene Adsorption on Pt Group Metals. <i>Journal of Physical Chemistry B</i> , 2006, 110, 17498-17506.	2.6	30
21	Overtone Vibrational Transition-Induced Lanthanide Excited-State Quenching in Yb ³⁺ /Er ³⁺ -Doped Upconversion Nanocrystals. <i>ACS Nano</i> , 2018, 12, 10572-10575.	14.6	29
22	A density functional theory approach to mushroom-like platinum clusters on palladium-shell over Au core nanoparticles for high electrocatalytic activity. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 5441.	2.8	28
23	Probing the Electronic Structure of Heterogeneous Metal Interfaces by Transition Metal Shelled Gold Nanoparticle-Enhanced Raman Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2016, 120, 20684-20691.	3.1	28
24	Theory for Modeling of High Resolution Resonant and Nonresonant Raman Images. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4986-4995.	5.3	24
25	Density functional theory study on the adsorption and decomposition of the formic acid catalyzed by highly active mushroom-like Au@Pd@Pt tri-metallic nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 4625.	2.8	22
26	Revisiting the Acetaldehyde Oxidation Reaction on a Pt Electrode by High-Sensitivity and Wide-Frequency Infrared Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 8727-8734.	4.6	21
27	Orientation Change of Adsorbed Pyrazine on Roughened Rhodium Electrodes as Probed by Surface-Enhanced Raman Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2005, 109, 17597-17602.	2.6	20
28	Bistability for CO Oxidation: An Understanding from Extended Phenomenological Kinetics Simulations. <i>ACS Catalysis</i> , 2019, 9, 11116-11124.	11.2	19
29	Hybrid molecular dynamics and first-principles study on the work function of a Pt(111) electrode immersed in aqueous solution at room temperature. <i>Physical Review B</i> , 2012, 86, .	3.2	18
30	Aggregation-induced chiral symmetry breaking of a naphthalimide-cyanostilbene dyad. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 23854-23860.	2.8	16
31	Optomagnetic Effect Induced by Magnetized Nanocavity Plasmon. <i>Journal of the American Chemical Society</i> , 2019, 141, 13795-13798.	13.7	16
32	Structures of Water Molecules Adsorbed on a Gold Electrode under Negative Potentials. <i>Journal of Physical Chemistry C</i> , 2010, 114, 4051-4056.	3.1	15
33	Significant Contributions of the Albrecht's A Term to Nonresonant Raman Scattering Processes. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5385-5390.	5.3	15
34	Molecular Design to Enhance the Thermal Stability of a Photo Switchable Molecular Junction Based on Dimethyldihydropyrene and Cyclophanediene Isomerization. <i>Journal of Physical Chemistry C</i> , 2015, 119, 11468-11474.	3.1	14
35	Lighting up long-range charge-transfer states by a localized plasmonic field. <i>Nanoscale</i> , 2017, 9, 18189-18193.	5.6	14
36	Identification of Water Hexamer on Cu(111) Surfaces. <i>Journal of the American Chemical Society</i> , 2020, 142, 6902-6906.	13.7	14

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37	Theoretical modeling of surface and tip-enhanced Raman spectroscopies. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2017, 7, e1293.	14.6	13
38	Quasi-Analytical Approach for Modeling of Surface-Enhanced Raman Scattering. <i>Journal of Physical Chemistry C</i> , 2015, 119, 28992-28998.	3.1	13
39	Vibrational identification for conformations of trans-1,2-bis (4-pyridyl) ethylene in gold molecular junctions. <i>Chemical Physics</i> , 2015, 453-454, 20-25.	1.9	12
40	Gauge invariant theory for super high resolution Raman images. <i>Journal of Chemical Physics</i> , 2017, 146, 194106.	3.0	12
41	Identifying the structure of 4-chlorophenyl isocyanide adsorbed on Au(111) and Pt(111) surfaces by first-principles simulations of Raman spectra. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 32389-32397.	2.8	12
42	Theoretical modeling of tip-enhanced resonance Raman images of switchable azobenzene molecules on Au(111). <i>Nanoscale</i> , 2018, 10, 11850-11860.	5.6	12
43	Molecular polarization bridging physical and chemical enhancements in surface enhanced Raman scattering. <i>Chemical Communications</i> , 2011, 47, 11438.	4.1	11
44	Optical Excitation in Donor-Acceptor Complexes: Role of the Structure. <i>Journal of Physical Chemistry A</i> , 2016, 120, 3547-3553.	2.5	11
45	Tuning electronic and magnetic properties of armchair zigzag hybrid graphene nanoribbons by the choice of supercell model of grain boundaries. <i>Journal of Applied Physics</i> , 2014, 115, 104303.	2.5	10
46	Monitoring Hydrogen/Deuterium Tautomerization in Transient Isomers of Single Porphine by Highly Localized Plasmonic Field. <i>Journal of Physical Chemistry C</i> , 2019, 123, 11081-11093.	3.1	9
47	Structural Phase Transitions of Molecular Self-Assembly Driven by Nonbonded Metal Adatoms. <i>ACS Nano</i> , 2020, 14, 6331-6338.	14.6	9
48	The effect of Duschinsky rotation on charge transport properties of molecular junctions in the sequential tunneling regime. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 23007-23016.	2.8	8
49	Structural Exploration of Multilayered Ionic Liquid/Ag Electrode Interfaces by Atomic Force Microscopy and Surface-Enhanced Raman Spectroscopy. <i>ChemElectroChem</i> , 2020, 7, 4936-4942.	3.4	8
50	Finding the true pathway for reversible isomerization of a single azobenzene molecule tumbling on Au(111) surface. <i>Nanoscale</i> , 2020, 12, 10474-10479.	5.6	8
51	Optical Images of Molecular Vibronic Couplings from Tip-Enhanced Fluorescence Excitation Spectroscopy. <i>Jacs Au</i> , 2022, 2, 150-158.	7.9	8
52	Theoretical simulations for vibrationally-resolved absorption spectra of naphthalenediimide cyclophane derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 183, 339-347.	3.9	7
53	Effects of Plasmon Modes on Resonant Raman Images of a Single Molecule. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 407-411.	4.6	7
54	Visualization of Vibrational Modes in Real Space by Tip-Enhanced Non-Resonant Raman Spectroscopy. <i>Angewandte Chemie</i> , 2016, 128, 1053-1057.	2.0	6

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55	Numerical investigations on the electromagnetic enhancement effect to tip-enhanced Raman scattering and fluorescence processes. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 235301.	1.8	6
56	Selective Catalytic Dehydrogenative Oxidation of Bio-Polyols to Lactic Acid. <i>Angewandte Chemie</i> , 2020, 132, 13975-13982.	2.0	6
57	Oxidation Mechanism of Si(111)-7 Å ² by Water: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 15763-15772.	3.1	4
58	Infrared spectra of small anionic water clusters from density functional theory and wavefunction theory calculations. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 12698-12707.	2.8	4
59	Electric Field Controlled Single-Molecule Optical Switch by Through-Space Charge Transfer State. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 9094-9099.	4.6	4
60	Thermal effects on electronic properties of CO/Pt(111) in water. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 13619.	2.8	2
61	Potential-Induced Phase Transition of <i>N</i> -Isobutyryl-L-cysteine Monolayers on Au (111) Surfaces. <i>Wuli Huaxue Xuebao/ Acta Physico-Chimica Sinica</i> , 2017, 33, 1010-1016.	4.9	2
62	Harvesting of surface plasmon polaritons: Role of the confinement factor. <i>Journal of Chemical Physics</i> , 2020, 153, 094107.	3.0	1
63	Surface-enhanced Raman Spectroscopy for Studying the Tensile Structure Between Au@Pd Nanoparticle Interfaces. , 2010, , .		0
64	Feasible Catalytic Strategy for Writing Conductive Nanoribbons on a Single-Layer Graphene Fluoride. <i>Journal of Physical Chemistry C</i> , 2014, 118, 22643-22648.	3.1	0
65	Visualization of Vibrational Modes in Real Space by Tip-Enhanced Non-Resonant Raman Spectroscopy (<i>Angew. Chem.</i> 3/2016). <i>Angewandte Chemie</i> , 2016, 128, 1232-1232.	2.0	0
66	Theoretical simulations of potential of zero charge for a Pt(111) electrode immersed in electrolyte solution with medium concentrations at room temperature. <i>Scientia Sinica Chimica</i> , 2015, 45, 1304-1309.	0.4	0