## Sai Duan

## List of Publications by Year in descending order

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257450 149698 3,257 66 24 56 citations h-index g-index papers 5091 68 68 68 citing authors all docs docs citations times ranked

#	Article	IF	CITATIONS
1	Optical Images of Molecular Vibronic Couplings from Tip-Enhanced Fluorescence Excitation Spectroscopy. Jacs Au, 2022, 2, 150-158.	7.9	8
2	Electric Field Controlled Single-Molecule Optical Switch by Through-Space Charge Transfer State. Journal of Physical Chemistry Letters, 2021, 12, 9094-9099.	4.6	4
3	Effects of Plasmon Modes on Resonant Raman Images of a Single Molecule. Journal of Physical Chemistry Letters, 2020, 11, 407-411.	4.6	7
4	Observation of inhomogeneous plasmonic field distribution in a nanocavity. Nature Nanotechnology, 2020, 15, 922-926.	31.5	62
5	Revisiting the Acetaldehyde Oxidation Reaction on a Pt Electrode by High-Sensitivity and Wide-Frequency Infrared Spectroscopy. Journal of Physical Chemistry Letters, 2020, 11, 8727-8734.	4.6	21
6	Harvesting of surface plasmon polaritons: Role of the confinement factor. Journal of Chemical Physics, 2020, 153, 094107.	3.0	1
7	Structural Exploration of Multilayered Ionic Liquid/Ag Electrode Interfaces by Atomic Force Microscopy and Surfaceâ€Enhanced Raman Spectroscopy. ChemElectroChem, 2020, 7, 4936-4942.	3.4	8
8	Selective Catalytic Dehydrogenative Oxidation of Bioâ€Polyols to Lactic Acid. Angewandte Chemie - International Edition, 2020, 59, 13871-13878.	13.8	39
9	Selective Catalytic Dehydrogenative Oxidation of Bioâ€Polyols to Lactic Acid. Angewandte Chemie, 2020, 132, 13975-13982.	2.0	6
10	Structural Phase Transitions of Molecular Self-Assembly Driven by Nonbonded Metal Adatoms. ACS Nano, 2020, 14, 6331-6338.	14.6	9
11	Exceeding the volcano relationship in oxygen reduction/evolution reactions using single-atom-based catalysts with dual-active-sites. Journal of Materials Chemistry A, 2020, 8, 10193-10198.	10.3	33
12	Real-time detection of single-molecule reaction by plasmon-enhanced spectroscopy. Science Advances, 2020, 6, eaba6012.	10.3	41
13	Identification of Water Hexamer on $Cu(111)$ Surfaces. Journal of the American Chemical Society, 2020, 142, 6902-6906.	13.7	14
14	Coreâ€"Shell Nanostructure-Enhanced Raman Spectroscopy for Surface Catalysis. Accounts of Chemical Research, 2020, 53, 729-739.	15.6	136
15	Microphotoelectrochemical Surface-Enhanced Raman Spectroscopy: Toward Bridging Hot-Electron Transfer with a Molecular Reaction. Journal of the American Chemical Society, 2020, 142, 8483-8489.	13.7	31
16	Finding the true pathway for reversible isomerization of a single azobenzene molecule tumbling on Au(111) surface. Nanoscale, 2020, 12, 10474-10479.	5.6	8
17	Optomagnetic Effect Induced by Magnetized Nanocavity Plasmon. Journal of the American Chemical Society, 2019, 141, 13795-13798.	13.7	16
18	Bistability for CO Oxidation: An Understanding from Extended Phenomenological Kinetics Simulations. ACS Catalysis, 2019, 9, 11116-11124.	11.2	19

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19	Atomically dispersed platinum supported on curved carbon supports for efficient electrocatalytic hydrogen evolution. Nature Energy, 2019, 4, 512-518.	39.5	756
20	Numerical investigations on the electromagnetic enhancement effect to tip-enhanced Raman scattering and fluorescence processes. Journal of Physics Condensed Matter, 2019, 31, 235301.	1.8	6
21	Monitoring Hydrogen/Deuterium Tautomerization in Transient Isomers of Single Porphine by Highly Localized Plasmonic Field. Journal of Physical Chemistry C, 2019, 123, 11081-11093.	3.1	9
22	Mechanism for the Extremely Efficient Sensitization of Yb <sup>3+</sup> Luminescence in CsPbCl <sub>3</sub> Nanocrystals. Journal of Physical Chemistry Letters, 2019, 10, 487-492.	4.6	55
23	Beyond Mean-Field Microkinetics: Toward Accurate and Efficient Theoretical Modeling in Heterogeneous Catalysis. ACS Catalysis, 2018, 8, 5816-5826.	11.2	41
24	Overtone Vibrational Transition-Induced Lanthanide Excited-State Quenching in Yb <sup>3+</sup> /Er <sup>3+</sup> -Doped Upconversion Nanocrystals. ACS Nano, 2018, 12, 10572-10575.	14.6	29
25	Theoretical modeling of tip-enhanced resonance Raman images of switchable azobenzene molecules on Au(111). Nanoscale, 2018, 10, 11850-11860.	<b>5.</b> 6	12
26	Theoretical modeling of surface and tipâ€enhanced Raman spectroscopies. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1293.	14.6	13
27	Theoretical simulations for vibrationally-resolved absorption spectra of naphthalenediimide cyclophane derivatives. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 183, 339-347.	3.9	7
28	Gauge invariant theory for super high resolution Raman images. Journal of Chemical Physics, 2017, 146, 194106.	3.0	12
29	Lighting up long-range charge-transfer states by a localized plasmonic field. Nanoscale, 2017, 9, 18189-18193.	5 <b>.</b> 6	14
30	Identifying the structure of 4-chlorophenyl isocyanide adsorbed on Au(111) and Pt(111) surfaces by first-principles simulations of Raman spectra. Physical Chemistry Chemical Physics, 2017, 19, 32389-32397.	2.8	12
31	Potential-Induced Phase Transition of $\langle i \rangle N \langle i \rangle$ -Isobutyryl-L-cysteine Monolayers on Au (111) Surfaces. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2017, 33, 1010-1016.	4.9	2
32	Visualization of Vibrational Modes in Real Space by Tipâ€Enhanced Nonâ€Resonant Raman Spectroscopy. Angewandte Chemie - International Edition, 2016, 55, 1041-1045.	13.8	46
33	Rù⁄4cktitelbild: Visualization of Vibrational Modes in Real Space by Tipâ€Enhanced Nonâ€Resonant Raman Spectroscopy (Angew. Chem. 3/2016). Angewandte Chemie, 2016, 128, 1232-1232.	2.0	0
34	Probing the Electronic Structure of Heterogeneous Metal Interfaces by Transition Metal Shelled Gold Nanoparticle-Enhanced Raman Spectroscopy. Journal of Physical Chemistry C, 2016, 120, 20684-20691.	3.1	28
35	Optical Excitation in Donor–Pt–Acceptor Complexes: Role of the Structure. Journal of Physical Chemistry A, 2016, 120, 3547-3553.	2.5	11
36	Theory for Modeling of High Resolution Resonant and Nonresonant Raman Images. Journal of Chemical Theory and Computation, 2016, 12, 4986-4995.	<b>5.</b> 3	24

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37	Visualization of Vibrational Modes in Real Space by Tipâ€Enhanced Nonâ€Resonant Raman Spectroscopy. Angewandte Chemie, 2016, 128, 1053-1057.	2.0	6
38	Molecular Design to Enhance the Thermal Stability of a Photo Switchable Molecular Junction Based on Dimethyldihydropyrene and Cyclophanediene Isomerization. Journal of Physical Chemistry C, 2015, 119, 11468-11474.	3.1	14
39	The effect of Duschinsky rotation on charge transport properties of molecular junctions in the sequential tunneling regime. Physical Chemistry Chemical Physics, 2015, 17, 23007-23016.	2.8	8
40	Theoretical Modeling of Plasmon-Enhanced Raman Images of a Single Molecule with Subnanometer Resolution. Journal of the American Chemical Society, 2015, 137, 9515-9518.	13.7	92
41	Infrared spectra of small anionic water clusters from density functional theory and wavefunction theory calculations. Physical Chemistry Chemical Physics, 2015, 17, 12698-12707.	2.8	4
42	Vibrational identification for conformations of trans-1,2-bis (4-pyridyl) ethylene in gold molecular junctions. Chemical Physics, 2015, 453-454, 20-25.	1.9	12
43	Significant Contributions of the Albrecht's <i>A</i> Term to Nonresonant Raman Scattering Processes. Journal of Chemical Theory and Computation, 2015, 11, 5385-5390.	5.3	15
44	Quasi-Analytical Approach for Modeling of Surface-Enhanced Raman Scattering. Journal of Physical Chemistry C, 2015, 119, 28992-28998.	3.1	13
45	Theoretical simulations of potential of zero charge for a Pt(111) electrode immersed in electrolyte solution with medium concentra-tions at room temperature. Scientia Sinica Chimica, 2015, 45, 1304-1309.	0.4	0
46	Tuning electronic and magnetic properties of armchair   zigzag hybrid graphene nanoribbons by the choice of supercell model of grain boundaries. Journal of Applied Physics, 2014, 115, 104303.	2.5	10
47	Aggregation-induced chiral symmetry breaking of a naphthalimide–cyanostilbene dyad. Physical Chemistry Chemical Physics, 2014, 16, 23854-23860.	2.8	16
48	Feasible Catalytic Strategy for Writing Conductive Nanoribbons on a Single-Layer Graphene Fluoride. Journal of Physical Chemistry C, 2014, 118, 22643-22648.	3.1	0
49	Roles of Plasmonic Excitation and Protonation on Photoreactions of <i>p</i> -Aminobenzenethiol on Ag Nanoparticles. Journal of Physical Chemistry C, 2014, 118, 6893-6902.	3.1	33
50	The Realistic Domain Structure of As-Synthesized Graphene Oxide from Ultrafast Spectroscopy. Journal of the American Chemical Society, 2013, 135, 12468-12474.	13.7	64
51	Thermal effects on electronic properties of CO/Pt(111) in water. Physical Chemistry Chemical Physics, 2013, 15, 13619.	2.8	2
52	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. Physical Chemistry Chemical Physics, 2013, 15, 4625.	2.8	22
53	Oxidation Mechanism of Si(111)-7 $\tilde{A}$ — 7 by Water: A Theoretical Study. Journal of Physical Chemistry C, 2013, 117, 15763-15772.	3.1	4
54	Hybrid molecular dynamics and first-principles study on the work function of a $Pt(111)$ electrode immersed in aqueous solution at room temperature. Physical Review B, 2012, 86, .	3.2	18

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55	A density functional theory approach to mushroom-like platinum clusters on palladium-shell over Au core nanoparticles for high electrocatalytic activity. Physical Chemistry Chemical Physics, 2011, 13, 5441.	2.8	28
56	Tailoring Au-core Pd-shell Pt-cluster nanoparticles for enhanced electrocatalytic activity. Chemical Science, 2011, 2, 531-539.	7.4	172
57	Molecular polarization bridging physical and chemical enhancements in surface enhanced Raman scattering. Chemical Communications, 2011, 47, 11438.	4.1	11
58	Surface-enhanced Raman Spectroscopy for Studying the Tensile Structure Between Au@Pd Nanoparticle Interfaces. , 2010, , .		0
59	SERS and DFT study of water on metal cathodes of silver, gold and platinum nanoparticles. Physical Chemistry Chemical Physics, 2010, 12, 2493.	2.8	73
60	Structures of Water Molecules Adsorbed on a Gold Electrode under Negative Potentials. Journal of Physical Chemistry C, 2010, 114, 4051-4056.	3.1	15
61	Epitaxial Growth of Heterogeneous Metal Nanocrystals: From Gold Nano-octahedra to Palladium and Silver Nanocubes. Journal of the American Chemical Society, 2008, 130, 6949-6951.	13.7	719
62	Chemical Enhancement Effects in SERS Spectra:  A Quantum Chemical Study of Pyridine Interacting with Copper, Silver, Gold and Platinum Metals. Journal of Physical Chemistry C, 2008, 112, 4195-4204.	3.1	207
63	Theoretical Study of Binding Interactions and Vibrational Raman Spectra of Water in Hydrogen-Bonded Anionic Complexes:  (H <sub>2</sub> O) <i><sub>n</sub></i> <sup>-</sup> ( <i>n</i> ) = 2)	Tj.ETQq1 :	1 <sub>.55</sub> 784314
64	Effect of Intrinsic Properties of Metals on the Adsorption Behavior of Molecules:Â Benzene Adsorption on Pt Group Metals. Journal of Physical Chemistry B, 2006, 110, 17498-17506.	2.6	30
65	Density functional theory study of surface-enhanced Raman scattering spectra of pyridine adsorbed on noble and transition metal surfaces. Journal of Raman Spectroscopy, 2005, 36, 533-540.	2.5	54
66	Orientation Change of Adsorbed Pyrazine on Roughened Rhodium Electrodes as Probed by Surface-Enhanced Raman Spectroscopy. Journal of Physical Chemistry B, 2005, 109, 17597-17602.	2.6	20