Jia Wang

List of Publications by Year
in descending order

130	3,586	279487 23	143772 57
papers	citations	h-index	g-index

132	132	132	5084
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantum tunneling of hydrogen atom transfer affects mandrel degradation in inertial confinement fusion target fabrication. IScience, 2022, 25, 103674.	1.9	4
2	Formation of twelve-fold iodine coordination at high pressure. Nature Communications, 2022, 13, 412.	5.8	23
3	Adatom Defect Induced Spin Polarization of Asymmetric Structures. ChemistryOpen, 2022, 11, e202100208.	0.9	1
4	High-Stability Light-Element Magnetic Superatoms Determined by Hundâ€™s Rule. Journal of Physical Chemistry Letters, 2022, 13, 2632-2637.	2.1	4
5	Tunable Spin Polarization of Zigzagâ€“Zigzag Heterojunction Carbon Nanotubes. Physica Status Solidi (B): Basic Research, 2022, 259, 2100639.	0.7	0
6	Magnetic coupling induced by the interaction between endohedral metal borofullerenes. RSC Advances, 2022, 12, 13401-13405.	1.7	1
7	Direct assembly between closed-shell coinage metal superatoms. Nano Research, 2022, 15, 8665-8672.	5.8	6
8	Initiator enhancement of mandrel degradation for ICF target fabrication. IScience, 2022, , 104733.	1.9	0
9	Constructing the bonding interactions between endohedral metallofullerene superatoms by embedded atomic regulation. Physical Chemistry Chemical Physics, 2021, 23, 15899-15903.	1.3	3
10	Mandrel degradation model of combined fast and slow processes. High Power Laser Science and Engineering, 2021, 9, .	2.0	5
11	Uncooperative Effect of Hydrogen Bond on Water Dimer. Chinese Physics Letters, 2021, 38, 013101.	1.3	6
12	Fully Active Nitrogen Energetic Chains Mg 2 (N 5) 2 N 2 [Mg 2 (N 5) 2 N 2] n under Ambient Conditions. Advanced Theory and Simulations, 2021, 4, 2000283.	1.3	2
13	Molecular insertion regulates the donor-acceptor interactions in cocrystals for the design of piezochromic luminescent materials. Nature Communications, 2021, 12, 4084.	5.8	41
14	A short-range disordered defect in the double layer ice. Journal of Molecular Liquids, 2021, 336, 116356.	2.3	1
15	A Covalentâ€Like Feature of Intermolecular Hydrogen Bonding in Energetic Molecules 3,6â€Dihydrazinoâ€sâ€tetrazine (DHT). Advanced Theory and Simulations, 2021, 4, 2100179.	1.3	2
16	Charge â€œSkin Behaviorâ€•of Gold Superatoms. Journal of Physical Chemistry Letters, 2021, 12, 8713-8719.	2.1	10
17	Pauli Repulsion Enhances Mobility of Ultraconfined Water. ACS Nano, 2021, 15, 2490-2496.	7.3	11
18	A Step-by-Step Process-Induced Unidirectional Oriented Water Wire in the Nanotube. Journal of Physical Chemistry Letters, 2021, 12, 350-354.	2.1	5

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19	Superatomic Rydberg State Excitation. Journal of Physical Chemistry Letters, 2021, , 11766-11771.	2.1	8
20	Adsorption enhanced photocatalytic degradation sulfadiazine antibiotic using porous carbon nitride nanosheets with carbon vacancies. Chemical Engineering Journal, 2020, 382, 123017.	6.6	83
21	Understanding the Hydrogen-Bonded Clusters of Ammonia (NH₃)_n (n = 3â€“6): Insights from the Electronic Structure Theory. ACS Omega, 2020, 5, 31724-31729.	1.6	10
22	Interaction potential energy surface between superatoms. Chemical Communications, 2020, 56, 14681-14684.	2.2	10
23	Intramolecular bonding properties in actinide embedded nearly planar superatoms. Chemical Physics Letters, 2020, 752, 137574.	1.2	4
24	Electronic Transport Inhibiting of Carbon Nanotubes by 5f Elements. Advanced Theory and Simulations, 2020, 3, 1900226.	1.3	2
25	High-Angular-Momentum Orbitals and Superatomic Characteristics of Boron-Nitrogen Cages. Journal of Physical Chemistry C, 2020, 124, 3881-3885.	1.5	9
26	Bonding properties of a superatom system with high-Z elements: insights from energy decomposition analysis. RSC Advances, 2020, 10, 14482-14486.	1.7	2
27	Superatomic physics: A new direction in atomic-level physics. Chinese Science Bulletin, 2020, 65, 2196-2200.	0.4	2
28	Zero-point fluctuation of hydrogen bond in water dimer from ab initio molecular dynamics. Chinese Physics B, 2020, 29, 103101.	0.7	1
29	Intermolecular vibrational energy transfers in nitro-energetic molecules: A first-principles molecular dynamics study. Chemical Physics Letters, 2019, 733, 136675.	1.2	1
30	The Reliability of the Densityâ€Functional Theory in Actinide Endohedral Systems. Advanced Theory and Simulations, 2019, 2, 1900138.	1.3	8
31	The nature of small molecules adsorbed on defective carbon nanotubes. Royal Society Open Science, 2019, 6, 190727.	1.1	7
32	An effective method to make polymers degrade readily: spatial isomerization. Physical Chemistry Chemical Physics, 2019, 21, 16905-16909.	1.3	4
33	Infrared spectral-shift induced by hydrogen bonding cooperativity in cyclic and prismatic water clusters. Journal of Molecular Liquids, 2019, 286, 110940.	2.3	5
34	Magnetic Coupling Induced Self-Assembly at Atomic Level[*]. Chinese Physics Letters, 2019, 36, 116401.	1.3	14
35	Superatom-assembly induced transition from insulator to semiconductor: A theoretical study. Science China Materials, 2019, 62, 416-422.	3.5	10
36	Tuning the functional groups of a graphene oxide membrane by Â·OH contributes to the nearly complete prevention of membrane fouling. Journal of Membrane Science, 2019, 576, 190-197.	4.1	14

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37	Dependence of characteristic interlayer vibration modes on interlayer spin arrangement in stacked graphene nanofragments. Carbon, 2019, 141, 339-347.	5.4	2
38	Spin polarization and dispersion effects in emergence of roaming transition state for nitrobenzene isomerization. Chinese Physics B, 2018, 27, 013102.	0.7	3
39	The electron density delocalization of hydrogen bond systems. Advances in Physics: X, 2018, 3, 1428915.	1.5	29
40	Localizationâ€vsâ€Delocalization of 5f Orbitals in Superatom Systems. Advanced Theory and Simulations, 2018, 1, 1700038.	1.3	7
41	The Dissociation Mechanism of Polyâ€Î±â€methylstyrene (PAMS) Dimers Induced by Spin Polarization. ChemistrySelect, 2018, 3, 2553-2557.	0.7	1
42	Emerging disciplines based on superatoms: a perspective point of view. Science Bulletin, 2018, 63, 395-397.	4.3	7
43	Hydrogen bonding cooperation in glycineâ€(water)_n clusters studied by density functional theory calculations. International Journal of Quantum Chemistry, 2018, 118, e25556.	1.0	0
44	Actinide endohedral boron clusters: A closed-shell electronic structure of U@B40. Nano Research, 2018, 11, 354-359.	5.8	35
45	Actinide embedded nearly planar gold superatoms: structural properties and applications in surface-enhanced Raman scattering (SERS). Physical Chemistry Chemical Physics, 2018, 20, 27523-27527.	1.3	14
46	Binding for endohedral-metallofullerene superatoms induced by magnetic coupling. Chemical Communications, 2018, 54, 13383-13386.	2.2	15
47	Altered superatomic properties of U@C28 by the electron rearrangement via adatom defects. Chemical Physics Letters, 2018, 712, 20-24.	1.2	3
48	Effect of confinement on water rotation via quantum tunnelling. Nanoscale, 2018, 10, 18622-18626.	2.8	6
49	The Effect of Polymer Structures on Complete Degradation: A Firstâ€Principles Study. ChemistryOpen, 2018, 7, 463-466.	0.9	5
50	Surfactant-Free Preparation of Au@Resveratrol Hollow Nanoparticles with Photothermal Performance and Antioxidant Activity. ACS Applied Materials & Interfaces, 2017, 9, 3376-3387.	4.0	35
51	Effect of Chain Conformation on the Single-Molecule Melting Force in Polymer Single Crystals: Steered Molecular Dynamics Simulations Study. Langmuir, 2017, 33, 1826-1833.	1.6	12
52	Quantitative contribution of molecular orbitals to hydrogen bonding in a water dimer: Electron density projected integral (EDPI) analysis. Chemical Physics Letters, 2017, 678, 98-101.	1.2	5
53	Unusual spin-polarized electron state in fullerene induced by carbon adatom defect. Nanoscale, 2017, 9, 7875-7879.	2.8	4
54	Theoretical study on electronic and vibrational properties of hydrogen bonds in glycine-water clusters. Chemical Physics Letters, 2017, 684, 53-59.	1.2	17

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55	Energetics competition in centrally four-coordinated water clusters and Raman spectroscopic signature for hydrogen bonding. RSC Advances, 2017, 7, 11680-11683.	1.7	21
56	First-principles study on charge transfer in an actinide-containing superatom from surface-enhanced Raman scattering. Journal of Materials Chemistry C, 2017, 5, 803-806.	2.7	10
57	Engineering a red emission of copper nanocluster self-assembly architectures by employing aromatic thiols as capping ligands. Nanoscale, 2017, 9, 12618-12627.	2.8	87
58	Cooperative vibrational properties of hydrogen bonds in Watsonâ€“Crick DNA base pairs. New Journal of Chemistry, 2017, 41, 12104-12109.	1.4	7
59	The synthesis and electrical transport of ligand-protected Au13 clusters. European Physical Journal D, 2017, 71, 1.	0.6	6
60	All-boron fullerene B40: a superatomic structure. Science China Materials, 2017, 60, 1264-1268.	3.5	12
61	Structural Asymmetry-Facilitated Tunability of Spin Distribution in the (10, 0) Carbon Nanotube Induced by Charging. Journal of Electronic Materials, 2017, 46, 3857-3861.	1.0	2
62	The selfâ€consistent charge density functional tightâ€binding theory study of carbon adatoms using tuned Hubbard U parameters. International Journal of Quantum Chemistry, 2017, 117, e25320.	1.0	1
63	Structural Influence on Superatomic Orbitals of Typical Gold Nanostructure Building Blocks. Journal of Electronic Materials, 2017, 46, 3938-3941.	1.0	5
64	Chemical Coupling SERS Properties of Pyridine on Silver-Caged Metal Clusters M@Ag12 (MÂ=ÂVâˆ', Nbâˆ',) Tj ETQq0 0 0 rgBT /Overlock	1.0	4
65	Spin Transfer in Polymer Degradation of Abnormal Linkage. Journal of Electronic Materials, 2017, 46, 3933-3937.	1.0	2
66	Ce@Au14: A Bimetallic Superatom Cluster with 18-Electron Rule. Journal of Electronic Materials, 2017, 46, 3899-3903.	1.0	7
67	Actinide-embedded gold superatom models: Electronic structure, spectroscopic properties, and applications in surface-enhanced Raman scattering. Nano Research, 2016, 9, 622-632.	5.8	38
68	Effects of 5f-elements on electronic structures and spectroscopic properties of gold superatom model. Chinese Physics B, 2016, 25, 083102.	0.7	16
69	Chirality recognition in concerted proton transfer process for prismatic water clusters. Nano Research, 2016, 9, 2782-2795.	5.8	17
70	Molecular orbital analysis of the hydrogen bonded water dimer. Scientific Reports, 2016, 6, 22099.	1.6	45
71	First Principles Study of the Interaction of Rare Gases in a U@C₆₀ Fullerene. ChemistrySelect, 2016, 1, 5624-5627.	0.7	4
72	Nonresonant chemical mechanism in surface-enhanced Raman scattering of pyridine on M@Au₁₂clusters. Nanoscale, 2016, 8, 4086-4093.	2.8	30

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73	High stability of the He atom confined in a U@C₆₀ fullerene. RSC Advances, 2016, 6, 29288-29293.	1.7	3
74	Chirality dependent spin polarization of carbon nanotubes. New Journal of Physics, 2016, 18, 023029.	1.2	8
75	First-Principles Calculations of Magnetism in Nanoscale Carbon Materials Confining Metal with f Valence Electrons. Journal of Cluster Science, 2016, 27, 845-860.	1.7	9
76	Depolymerization of Freeâ€Radical Polymers with Spin Migrations. ChemPhysChem, 2015, 16, 3308-3312.	1.0	11
77	Graphitic Carbon Nitride Polymers toward Sustainable Photoredox Catalysis. Angewandte Chemie - International Edition, 2015, 54, 12868-12884.	7.2	1,223
78	A strong charge-transfer effect in surface-enhanced Raman scattering induced by valence electrons of actinide elements. RSC Advances, 2015, 5, 32198-32204.	1.7	23
79	Enhancement of spin polarization induced by Coulomb on-site repulsion between localized pz electrons in graphene embedded with line defects. Physical Chemistry Chemical Physics, 2015, 17, 30744-30750.	1.3	5
80	Electronic delocalization in small water rings. Physical Chemistry Chemical Physics, 2015, 17, 2987-2990.	1.3	18
81	Correlation between electron delocalization and structural planarization in small water rings. International Journal of Quantum Chemistry, 2015, 115, 817-819.	1.0	5
82	Tunable dipole induced hydrogen bonds between a hydrogen molecule and alkali halides. Physical Chemistry Chemical Physics, 2015, 17, 20361-20367.	1.3	3
83	Strong Core@Shell Dependence in Surface-Enhanced Raman Scattering of Pyridine on Stable 13-Atom Silver-Caged Bimetallic Clusters. Journal of Physical Chemistry C, 2015, 119, 17429-17437.	1.5	19
84	Slippage in stacking of graphene nanofragments induced by spin polarization. Scientific Reports, 2015, 5, 10985.	1.6	9
85	A Study of Adsorption Behavior of Single Water Molecule on the Surface of Polyhedral Oligomeric Silsesquioxanes. Journal of Cluster Science, 2015, 26, 541-550.	1.7	1
86	Water film inside graphene nanosheets: electron transfer reversal between water and graphene via tight nano-confinement. RSC Advances, 2015, 5, 274-280.	1.7	17
87	Charging-induced asymmetric spin distribution in an asymmetric (9,0) carbon nanotube. Physical Chemistry Chemical Physics, 2015, 17, 28860-28865.	1.3	6
88	Assembly-Induced Enhancement of Cu Nanoclusters Luminescence with Mechanochromic Property. Journal of the American Chemical Society, 2015, 137, 12906-12913.	6.6	367
89	U@C₂₈: the electronic structure induced by the 32-electron principle. Physical Chemistry Chemical Physics, 2015, 17, 23308-23311.	1.3	40
90	Structural and electronic properties of uranium-encapsulated Au14 cage. Scientific Reports, 2015, 4, 5862.	1.6	29

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91	Environmental-Confinement-Induced Stability Enhancement of Chiral Molecules. ChemPhysChem, 2014, 15, 2672-2675.	1.0	0
92	The ground state and electronic structure of Gd@C82: A systematic theoretical investigation of first principle density functionals. Journal of Chemical Physics, 2014, 141, 244306.	1.2	22
93	A unique feature of chiral transition of a difluorobenzo[c]phenanthrene molecule confined in a boron-nitride nanotube based on molecular dynamics simulations. Chemical Physics Letters, 2014, 591, 265-267.	1.2	5
94	Defect-induced strong localization of uranium dicarbide on the graphene surface. Physical Chemistry Chemical Physics, 2014, 16, 22784-22790.	1.3	16
95	Effect of ligands on the characteristics of (CdSe)₁₃quantum dots. RSC Advances, 2014, 4, 27146-27151.	1.7	23
96	The mechanism of Nâ€“Ag bonding determined tunability of surface-enhanced Raman scattering of pyridine on MAg (M = Cu, Ag, Au) diatomic clusters. Physical Chemistry Chemical Physics, 2014, 16, 20665-20671.	1.3	21
97	De Novo Design of an Endohedral Heteronuclear Dimetallofullerene (Uï£¿Gd)@C₆₀ with Exceptional Structural and Electronic Properties. ChemPhysChem, 2014, 15, 3871-3876.	1.0	10
98	Stable electronic structures of a defective uranofullerene. Carbon, 2014, 78, 19-25.	5.4	11
99	Carbon nanotubes adsorb U atoms differently in their inner and outer surfaces. RSC Advances, 2014, 4, 30074.	1.7	10
100	Dual Inhibitory Pathways of Metallofullerenol Gd@C82(OH)22 on Matrix Metalloproteinase-2: Molecular insight into drug-like nanomedicine. Scientific Reports, 2014, 4, 4775.	1.6	25
101	Anomalous stability of graphene containing defects covered by a water layer. Nanoscale, 2013, 5, 6767.	2.8	12
102	Basis set effect on defect induced spin polarization of a carbon nanotube in density functional theory calculations. Chemical Physics Letters, 2013, 585, 107-111.	1.2	4
103	Signatures in vibrational and UV-visible absorption spectra for identifying cyclic hydrocarbons by graphene fragments. Nanoscale, 2013, 5, 12178.	2.8	15
104	Strong Adsorption Between Uranium Dicarbide and Graphene Surface Induced by f Electrons. Journal of Physical Chemistry C, 2013, 117, 26849-26857.	1.5	14
105	Adsorptive separation of ethylene/ethane mixtures using carbon nanotubes: a molecular dynamics study. Journal Physics D: Applied Physics, 2013, 46, 395302.	1.3	12
106	Structure, magnetic, and electronic properties of hydrogenated two-dimensional diamond films. Applied Physics Letters, 2013, 102, 073114.	1.5	30
107	Chemical Mechanism and Tunability of Surface-Enhanced Raman Scattering of Pyridine on Heteronuclear Coinage Metal Diatomic Clusters: A Density Functional Study. Journal of Physical Chemistry C, 2013, 117, 12544-12551.	1.5	16
108	Defect Induced Electronic Structure of Uranofullerene. Scientific Reports, 2013, 3, 1341.	1.6	30

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109	HYPERCONJUGATION EFFECT ON THE STRUCTURAL STABILITY OF A TERT-BUTYL AND ITS DERIVED C4Hn(n =) Tj ETQq1 1 0.784314 rgB	1.8	2
110	Energetics and Electronic Properties of a Neutral Diuranium Molecule Encapsulated in C90 Fullerene. Procedia Chemistry, 2012, 7, 528-533.	0.7	13
111	Enantiomerization Mechanism of Thalidomide and the Role of Water and Hydroxide Ions. Chemistry - A European Journal, 2012, 18, 14305-14313.	1.7	30
112	Density Functional Theoretical Analysis of the Molecular Structural Effects on Raman Spectra of Î²â€Carotene and Lycopene. Chinese Journal of Chemistry, 2012, 30, 2573-2580.	2.6	16
113	Layer number-dependent structural evolution of two-dimensional diamond films. Chemical Physics Letters, 2012, 550, 130-133.	1.2	30
114	Strong interactions and charge transfers between a charged benzene molecule and multilayer graphenes. Journal of Materials Chemistry, 2012, 22, 23380.	6.7	19
115	Characteristic Vibrational Modes and Electronic Structures of Carbon Nanotubes Containing Defects. Journal of Physical Chemistry C, 2012, 116, 292-297.	1.5	14
116	Amino acid analogues bind to carbon nanotube via Ï€-Ï€ interactions: Comparison of molecular mechanical and quantum mechanical calculations. Journal of Chemical Physics, 2012, 136, 025103.	1.2	103
117	Transformation mechanism of a H2 molecule from physisorption to chemisorption in pristine and B-doped C20 fullerenes. Chemical Physics Letters, 2011, 511, 393-398.	1.2	22
118	Adsorption of sodium ions and hydrated sodium ions on a hydrophobic graphite surface via cation-Ï€ interactions. Chinese Physics B, 2011, 20, 068101.	0.7	26
119	PHYSISORPTION TO CHEMISORPTION TRANSFORMATION OF A H2 MOLECULE ON B-DOPED FULLERENE C59B. Journal of Theoretical and Computational Chemistry, 2011, 10, 839-847.	1.8	5
120	Size Dependence of Nanoscale Confinement on Chiral Transformation. Chemistry - A European Journal, 2010, 16, 6482-6487.	1.7	6
121	Stable Liquid Water Droplet on a Water Monolayer Formed at Room Temperature on Ionic Model Substrates. Physical Review Letters, 2009, 103, 137801.	2.9	238
122	Theoretical study on the structures and dissociation processes of hexatomic sulphur. Computational and Theoretical Chemistry, 2009, 906, 1-5.	1.5	3
123	Effect of Î²-Ring Rotation on the Structures and Vibrational Spectra of Î²-Carotene: Density Functional Theory Analysis. Journal of Physical Chemistry A, 2008, 112, 10580-10585.	1.1	30
124	Raman signature to identify the structural transition of single-wall carbon nanotubes under high pressure. Physical Review B, 2008, 78, .	1.1	79
125	Anomalous pressure behavior of tangential modes in single-wall carbon nanotubes. Physical Review B, 2007, 76, .	1.1	12
126	A Barrierless Process from Physisorption to Chemisorption of H2 Molecules on Light-Element-Doped Fullerenes. Journal of Physical Chemistry C, 2007, 111, 4473-4476.	1.5	16

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127	Transient gain property of a weak probe field in an asymmetric semiconductor coupled double quantum well structure. Physics Letters, Section A: General, Atomic and Solid State Physics, 2007, 370, 113-118.	0.9	7
128	The two hydrogen transfer dissociation channels of nicotine molecule in the gas phase. Computational and Theoretical Chemistry, 2006, 767, 95-101.	1.5	2
129	A path from Ih to C1 symmetry for C20 cage molecule. Journal of Computational Chemistry, 2005, 26, 1279-1283.	1.5	8
130	Superatomic Rydberg State Excitation. SSRN Electronic Journal, 0, , .	0.4	0