Han-Shi Hu

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

68 papers	3,261 citations	26 h-index	57 g-index
73 ext. papers	3,802 ext. citations	8.7 avg, IF	5.15 L-index

#	Paper	IF	Citations
68	Infrared spectroscopic signature of the structural diversity of the water heptamer. *Cell Reports Physical Science*, **2022**, 3, 100748	6.1	3
67	Formation and Characterization of BeFe(CO) Anion with Beryllium-Iron Bonding. *Angewandte Chemie - International Edition*, **2021**, 60, 9334-9338	16.4	4
66	Formation and Characterization of BeFe(CO)4 Anion with Beryllium Iron Bonding. *Angewandte Chemie*, **2021**, 133, 9420-9424	3.6	0
65	Norm-Conserving Pseudopotentials and Basis Sets to Explore Actinide Chemistry in Complex Environments. *Journal of Chemical Theory and Computation*, **2021**, 17, 3360-3371	6.4	4
64	Atomically Dispersed Pt-NC Sites Enabling Efficient and Selective Electrocatalytic C-C Bond Cleavage in Lignin Models under Ambient Conditions. *Journal of the American Chemical Society*, **2021**, 143, 9429-9439	16.4	43
63	CoO-metalloxocubes: a new class of perovskite-like neutral clusters with cubic aromaticity. *National Science Review*, **2021**, 8, nwaa201	10.8	13
62	Ligands enhanced the Ac[triple bond, length as m-dash]Ac triple bond. *Physical Chemistry Chemical Physics*, **2021**, 23, 10244-10250	3.6	1
61	Construction of Dual-Active-Site Copper Catalyst Containing both Cu?N and Cu?N Sites. *Small*, **2021**, 17, e2006834	11	14
60	2-Butene Tetraanion Bridged Dinuclear Samarium(III) Complexes via Sm(II)-Mediated Reduction of Electron-Rich Olefins. *Journal of the American Chemical Society*, **2020**, 142, 10705-10714	16.4	9
59	Infrared spectroscopy of neutral water clusters at finite temperature: Evidence for a noncyclic pentamer. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 15423-15428	11.5	24
58	Multiple Bonding Between Group 3 Metals and Fe(CO)3 *Angewandte Chemie*, **2020**, 132, 2364-2368	3.6	0
57	Formation and Characterization of a BeOBeC Multiple Radical Featuring a Quartet Carbyne Moiety. *Angewandte Chemie - International Edition*, **2020**, 59, 6923-6928	16.4	9
56	Infrared Spectroscopy of Neutral Water Dimer Based on a Tunable Vacuum Ultraviolet Free Electron Laser. *Journal of Physical Chemistry Letters*, **2020**, 11, 851-855	6.4	22
55	Multiple Bonding Between Group 3 Metals and Fe(CO). *Angewandte Chemie - International Edition*, **2020**, 59, 2344-2348	16.4	9
54	Understanding the Uniqueness of 2p Elements in Periodic Tables. *Chemistry - A European Journal*, **2020**, 26, 15558-15564	4.8	17
53	Wet carbonate-promoted radical arylation of vinyl pinacolboronates with diaryliodonium salts yields substituted olefins. *Communications Chemistry*, **2020**, 3,	6.3	4
52	Infrared spectroscopic study of hydrogen bonding topologies in the smallest ice cube. *Nature Communications*, **2020**, 11, 5449	17.4	15

51	Distinct electronic structures and bonding interactions in inverse-sandwich samarium and ytterbium biphenyl complexes. *Chemical Science*, **2020**, 12, 227-238	9.4	6
50	Probing the electronic structure of the CoB16⁻ drum complex: Unusual oxidation state of Co. *Chinese Journal of Chemical Physics*, **2019**, 32, 241-247	0.9	3
49	The df-d Dative Bonding in a Uranium-Cobalt Heterobimetallic Complex for Efficient Nitrogen Fixation. *Inorganic Chemistry*, **2019**, 58, 7433-7439	5.1	9
48	Triple bonds between iron and heavier group-14 elements in the AFe(CO) complexes (A = Ge, Sn, and Pb). *Chemical Communications*, **2019**, 55, 5685-5688	5.8	13
47	High Uptake of ReO and CO Conversion by a Radiation-Resistant Thorium-Nickle [Th Ni] Nanocage-Based Metal-Organic Framework. *Angewandte Chemie - International Edition*, **2019**, 58, 6022-6027	16.4	77
46	An Ultrastable Matryoshka [Hf] Nanocluster as a Luminescent Sensor for Concentrated Alkali and Acid. *Angewandte Chemie - International Edition*, **2019**, 58, 16610-16616	16.4	26
45	An Ultrastable Matryoshka [Hf13] Nanocluster as a Luminescent Sensor for Concentrated Alkali and Acid. *Angewandte Chemie*, **2019**, 131, 16763-16769	3.6	4
44	Quadruple bonding between iron and boron in the BFe(CO) complex. *Nature Communications*, **2019**, 10, 4713	17.4	26
43	Physical origin of chemical periodicities in the system of elements. *Pure and Applied Chemistry*, **2019** , 91, 1969-1999	2.1	10
42	Lanthanides with Unusually Low Oxidation States in the PrB and PrB Boride Clusters. *Inorganic Chemistry*, **2019**, 58, 411-418	5.1	23
41	High Spin Ground States in Matryoshka Actinide Nanoclusters: A Computational Study. *Chemistry - A European Journal*, **2018**, 24, 347-350	4.8	4
40	Relativity-Induced Bonding Pattern Change in Coinage Metal Dimers M (M = Cu, Ag, Au, Rg). *Inorganic Chemistry*, **2018**, 57, 5499-5506	5.1	10
39	Recent Progress on the investigations of boron clusters and boron-based materials (I): borophene. *Scientia Sinica Chimica*, **2018**, 48, 98-107	1.6	10
38	Triple Bonds Between Iron and Heavier Group 15 Elements in AFe(CO) (A=As, Sb, Bi) Complexes. *Angewandte Chemie - International Edition*, **2018**, 57, 542-546	16.4	20
37	Stable Zn -Containing MOFs with Large [Zn] Nanocages from Assembly of Zn Ions and Aromatic [Zn] Clusters. *Chemistry - A European Journal*, **2018**, 24, 3683-3688	4.8	16
36	Post Hartree-Fock calculations of pnictogen-uranium bonding in EUF (E = N-Bi). *Chemical Communications*, **2018**, 54, 11100-11103	5.8	5
35	The shortest Th-Th distance from a new type of quadruple bond. *Physical Chemistry Chemical Physics*, **2017**, 19, 5070-5076	3.6	22
34	Relativistic Effects Break Periodicity in Group 6 Diatomic Molecules. *Journal of the American Chemical Society*, **2016**, 138, 1126-9	16.4	31

33	Theoretical studies of the global minima and polarizabilities of small lithium clusters. *Chemical Physics Letters*, **2016**, 644, 235-242	2.5	10
32	A multicentre-bonded [Zn(I)]8 cluster with cubic aromaticity. *Nature Communications*, **2015**, 6, 6331	17.4	73
31	Infrared multiphoton dissociation spectroscopy of a gas-phase complex of uranyl and 3-oxa-glutaramide: an extreme red-shift of the [O?U?O](2+) asymmetric stretch. *Journal of Physical Chemistry A*, **2015**, 119, 3366-74	2.8	18
30	Metal□Organic Frameworks (MOFs) of a Cubic Metal Cluster with Multicentered MnI?MnI Bonds. *Angewandte Chemie*, **2015**, 127, 11847-11851	3.6	9
29	Metal-Organic Frameworks (MOFs) of a Cubic Metal Cluster with Multicentered Mn(I)-Mn(I) Bonds. *Angewandte Chemie - International Edition*, **2015**, 54, 11681-5	16.4	36
28	Experimental and theoretical evidence of an axially chiral borospherene. *ACS Nano*, **2015**, 9, 754-60	16.7	195
27	[B□]?: a quasiplanar chiral boron cluster. *Angewandte Chemie - International Edition*, **2014**, 53, 5540-5	16.4	116
26	Strong electron correlation in UO2(-): a photoelectron spectroscopy and relativistic quantum chemistry study. *Journal of Chemical Physics*, **2014**, 140, 094306	3.9	23
25	Planar hexagonal B(36) as a potential basis for extended single-atom layer boron sheets. *Nature Communications*, **2014**, 5, 3113	17.4	503
24	Actinide-silicon multiradical bonding: infrared spectra and electronic structures of the Si(□X)AnF3 (An = Th, U; X = H, F) molecules. *Journal of the American Chemical Society*, **2014**, 136, 1427-37	16.4	37
23	Describing Excited State Relaxation and Localization in TiO2 Nanoparticles Using TD-DFT. *Journal of Chemical Theory and Computation*, **2014**, 10, 5538-48	6.4	29
22	The B35 cluster with a double-hexagonal vacancy: a new and more flexible structural motif for borophene. *Journal of the American Chemical Society*, **2014**, 136, 12257-60	16.4	250
21	[B30]□A Quasiplanar Chiral Boron Cluster. *Angewandte Chemie*, **2014**, 126, 5646-5651	3.6	28
20	Observation of an all-boron fullerene. *Nature Chemistry*, **2014**, 6, 727-31	17.6	590
19	Modeling Excited States in TiO Nanoparticles: On the Accuracy of a TD-DFT Based Description. *Journal of Chemical Theory and Computation*, **2014**, 10, 1189-1199	6.4	48
18	Ultrathin rhodium nanosheets. *Nature Communications*, **2014**, 5, 3093	17.4	350
17	Toward enabling large-scale open-shell equation-of-motion coupled cluster calculations: triplet states of □carotene. *Journal of Physical Chemistry A*, **2014**, 118, 9087-93	2.8	9
16	A tetrapositive metal ion in the gas phase: thorium(IV) coordinated by neutral tridentate ligands. *Angewandte Chemie - International Edition*, **2013**, 52, 6885-8	16.4	30

15	Experimental and theoretical studies on the fragmentation of gas-phase uranyl-, neptunyl-, and plutonyl-diglycolamide complexes. *Journal of Physical Chemistry A*, **2013**, 117, 10544-50	2.8	31
14	Excitation Energies with Cost-Reduced Variant of the Active-Space EOMCCSDT Method: The EOMCCSDt-3 Approach. *Journal of Chemical Theory and Computation*, **2013**, 9, 4761-8	6.4	2
13	Probing the electronic structures of low oxidation-state uranium fluoride molecules UF(x)- (x = 2-4). *Journal of Chemical Physics*, **2013**, 139, 244303	3.9	13
12	A Tetrapositive Metal Ion in the Gas Phase: Thorium(IV) Coordinated by Neutral Tridentate Ligands. *Angewandte Chemie*, **2013**, 125, 7023-7026	3.6	
11	On the maximum bond multiplicity of carbon: unusual C?U quadruple bonding in molecular CUO. *Chemical Science*, **2012**, 3, 2786	9.4	41
10	Matrix infrared spectroscopic and computational investigations of the lanthanide-methylene complexes CH2LnF2 with single Ln-C bonds. *Journal of Physical Chemistry A*, **2011**, 115, 1913-21	2.8	26
9	Chemisorption-Induced 2D→3D→2D Structural Transitions in Gold Heptamer: (CO)nAu7⁻ (n = 1→4). *Journal of Physical Chemistry Letters*, **2011**, 2, 2288-2293	6.4	26
8	Theoretical investigations on the formation and dehydrogenation reaction pathways of H(NH2BH2)(n)H (n = 1-4) oligomers: importance of dihydrogen interactions. *Inorganic Chemistry*, **2010**, 49, 7710-20	5.1	36
7	Theoretical investigations of geometry, electronic structure and stability of UO(6): octahedral uranium hexoxide and its isomers. *Journal of Physical Chemistry A*, **2010**, 114, 8837-44	2.8	36
6	Infrared spectra and electronic structures of agostic uranium methylidene molecules. *Inorganic Chemistry*, **2008**, 47, 1435-42	5.1	49
5	Infrared and DFT investigations of the XC[triple bond]ReX3 and HC[triple bond]ReX3 complexes: Jahn-Teller distortion and the methylidyne C-X(H) stretching absorptions. *Inorganic Chemistry*, **2007**, 46, 8728-38	5.1	20
4	Chirality, agostic interactions, and pyramidality in actinide methylidene complexes. *Angewandte Chemie - International Edition*, **2007**, 46, 9045-9	16.4	37
3	Chirality, Agostic Interactions, and Pyramidality in Actinide Methylidene Complexes. *Angewandte Chemie*, **2007**, 119, 9203-9207	3.6	9
2	Formation of unprecedented actinide triple bond carbon in uranium methylidyne molecules. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 18919-24	11.5	74
1	Computational Prediction of Graphdiyne-Supported Three-Atom Single-Cluster Catalysts. *CCS Chemistry*,1-24	7.2	1