Xiaoyan Cao

List of Publications by Year in descending order

48 papers	4,377 citations	218677 26 h-index	189892 50 g-index
52 all docs	52 docs citations	52 times ranked	3024 citing authors

#	Article	IF	Citations
1	Segmented contraction scheme for small-core lanthanide pseudopotential basis sets. Computational and Theoretical Chemistry, 2002, 581, 139-147.	1.5	653
2	Valence basis sets for relativistic energy-consistent small-core actinide pseudopotentials. Journal of Chemical Physics, 2003, 118, 487-496.	3.0	640
3	Segmented contraction scheme for small-core actinide pseudopotential basis sets. Computational and Theoretical Chemistry, 2004, 673, 203-209.	1.5	616
4	Valence basis sets for relativistic energy-consistent small-core lanthanide pseudopotentials. Journal of Chemical Physics, 2001, 115, 7348-7355.	3.0	574
5	Relativistic Pseudopotentials: Their Development and Scope of Applications. Chemical Reviews, 2012, 112, 403-480.	47.7	346
6	First-Principles Study of the Separation of Am^{III}/Cm^{III} from Eu^{III} with Cyanex301. Inorganic Chemistry, 2010, 49, 10307-10315.	4.0	119
7	Accurate Relativistic Small-Core Pseudopotentials for Actinides. Energy Adjustment for Uranium and First Applications to Uranium Hydride. Journal of Physical Chemistry A, 2009, 113, 12573-12581.	2.5	96
8	Computational study of lanthanide(iii) hydration. Physical Chemistry Chemical Physics, 2010, 12, 13215.	2.8	96
9	Approaching actinide(+III) hydration from first principles. Physical Chemistry Chemical Physics, 2007, 9, 459-465.	2.8	94
10	Quasirelativistic energy-consistent 5f-in-core pseudopotentials for trivalent actinide elements. Theoretical Chemistry Accounts, 2007, 117, 473-481.	1.4	88
11	Quasirelativistic f-in-core pseudopotentials and core-polarization potentials for trivalent actinides and lanthanides: molecular test for trifluorides. Theoretical Chemistry Accounts, 2010, 126, 117-127.	1.4	87
12	Quasirelativistic energy-consistent 5f-in-core pseudopotentials for divalent and tetravalent actinide elements. Theoretical Chemistry Accounts, 2007, 118, 845-854.	1.4	78
13	Relativistic energy-consistent ab initio pseudopotentials as tools for quantum chemical investigations of actinide systems. Coordination Chemistry Reviews, 2006, 250, 900-910.	18.8	66
14	Relativistic Small-Core Pseudopotentials for Actinium, Thorium, and Protactinium. Journal of Physical Chemistry A, 2014, 118, 2519-2530.	2.5	60
15	Theoretical prediction of the second to fourth actinide ionization potentials. Molecular Physics, 2003, 101, 961-969.	1.7	54
16	Accurate relativistic energy-consistent pseudopotentials for the superheavy elements 111 to 118 including quantum electrodynamic effects. Journal of Chemical Physics, 2012, 136, 214105.	3.0	53
17	The Origin of the Photoluminescence Enhancement of Goldâ€Đoped Silver Nanoclusters: The Importance of Relativistic Effects and Heteronuclear Goldâ€“Silver Bonds. Angewandte Chemie - International Edition, 2018, 57, 9965-9969.	13.8	53
18	Electronic structure of lanthanide dimers. Molecular Physics, 2003, 101, 1967-1976.	1.7	44

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19	Pseudopotential study of lanthanum and lutetium dimers. Theoretical Chemistry Accounts, 2002, 108, 143-149.	1.4	43
20	Accurate quantum chemical modelling of the separation of Eu³⁺from Am³⁺/Cm³⁺by liquidâ€“liquid extraction with Cyanex272. Physical Chemistry Chemical Physics, 2015, 17, 20605-20616.	2.8	41
21	Visibleâ€Light Photocatalysis of C(sp³)â€H Fluorination by the Uranyl Ion: Mechanistic Insights. Angewandte Chemie - International Edition, 2018, 57, 11812-11816.	13.8	40
22	Molecular structure of diatomic lanthanide compounds. Science in China Series B: Chemistry, 2002, 45, 91.	0.8	37
23	Pseudopotentials and modelpotentials. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 200-210.	14.6	37
24	Regulatory Mechanism of the Enantioselective Intramolecular Enone [2+2] Photocycloaddition Reaction Mediated by a Chiral Lewis Acid Catalyst Containing Heavy Atoms. Angewandte Chemie - International Edition, 2015, 54, 14295-14298.	13.8	35
25	Density Functional Theory Studies of Actinide(III) Motexafins (An-Motex2+, An = Ac, Cm, Lr). Structure, Stability, and Comparison with Lanthanide(III) Motexafins. Inorganic Chemistry, 2006, 45, 3444-3451.	4.0	30
26	Basis set limit extrapolation of ACPF and CCSD(T) results for the third and fourth lanthanide ionization potentials. Chemical Physics Letters, 2001, 349, 489-495.	2.6	28
27	Density functional studies on lanthanide (III) texaphyrins (Ln-Tex2+, Ln = La, Gd, Lu): structure, stability and electronic excitation spectrum. Molecular Physics, 2003, 101, 2427-2435.	1.7	26
28	Misleading evidence for covalent bonding from EuIIIX and AmIIIX density functional theory bond lengths. Journal of Electron Spectroscopy and Related Phenomena, 2014, 194, 8-13.	1.7	26
29	Energy Resonance Crossing Controls the Photoluminescence of Europium Antenna Probes. Angewandte Chemie - International Edition, 2017, 56, 7986-7990.	13.8	23
30	Relativistic Pseudopotentials. Challenges and Advances in Computational Chemistry and Physics, 2010, , 215-277.	0.6	23
31	Multiconfiguration Diracâ^'Hartreeâ^'Fock Adjusted Energy-Consistent Pseudopotential for Uranium: Spinâ^'Orbit Configuration Interaction and Fock-Space Coupled-Cluster Study of U⁴⁺ and U⁵⁺. Journal of Physical Chemistry A, 2009, 113, 11509-11516.	2.5	20
32	Electron affinity of Ce and electronic states ofCeâ^'. Physical Review A, 2004, 69, .	2.5	18
33	All-electron Douglasâ€“Krollâ€“Hess and pseudopotential study on the low-lying states of uranium hydride UH. Chemical Physics, 2008, 343, 250-257.	1.9	17
34	THE RELATIVISTIC ENERGY-CONSISTENT AB INITIO PSEUDOPOTENTIAL APPROACH AND ITS APPLICATION TO LANTHANIDE AND ACTINIDE COMPOUNDS. Recent Advances in Computational, 2004, , 1-35.	0.8	16
35	Density Functional Studies of Coenzyme NADPH and Its Oxidized Form NADP+: Structures, UVâ€“Vis Spectra, and the Oxidation Mechanism of NADPH. Journal of Computational Chemistry, 2020, 41, 305-316.	3.3	13
36	PSEUDOPOTENTIAL STUDIES ON THE ELECTRONIC STRUCTURE OF LANTHANUM MONOHALIDES LaF, LaCl, LaBr, AND LaI. Journal of Theoretical and Computational Chemistry, 2005, 04, 583-592.	1.8	12

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37	Ab initio studies on the electronic structure of FeOH. Chemical Physics, 2005, 311, 203-208.	1.9	10
38	HeI photoelectron spectroscopic study of the electronic structure of SSF2 and FSSF compounds. Chemical Physics Letters, 1998, 290, 405-408.	2.6	9
39	A kinetic study of the isomerization reaction from SSF2 to FSSF using the HeI photoelectron spectroscopic method. Chemical Physics Letters, 1999, 299, 322-326.	2.6	9
40	The first water coordination sphere of lanthanide(iii) motexafins (Ln-Motex2+, Ln = La, Gd, Lu) and its effects on structures, reduction potentials and UV-vis absorption spectra. Theoretical studies. Physical Chemistry Chemical Physics, 2017, 19, 20160-20171.	2.8	9
41	Ursache der PhotolumineszenzverstÃrkung in Goldâ€dotierten Silberâ€Nanoclustern: BeitrÃge relativistischer Effekte und heteronuklearer Goldâ€Silberâ€Bindungen. Angewandte Chemie, 2018, 130, 10114-10119.	2.0	6
42	Quantum chemical study of the autoxidation of ascorbate. Journal of Computational Chemistry, 2016, 37, 1914-1923.	3.3	4
43	Energieresonanzkreuzung steuert die Photolumineszenz von Europiumâ€Antennensonden. Angewandte Chemie, 2017, 129, 8097-8101.	2.0	4
44	Photokatalyse der C(sp³)â€Hâ€Fluorierung durch Uranyl mit sichtbarem Licht: Einblicke in den Mechanismus. Angewandte Chemie, 2018, 130, 11986-11990.	2.0	4
45	New Basis Sets for Lanthanide and Actinide Energyâ€consistent Smallâ€core Pseudopotentials. Journal of the Chinese Chemical Society, 2003, 50, 665-676.	1.4	3
46	HeI photoelectron spectroscopic (PES) and quantum chemistry study on the dimeric compound of 2(5H) furanone. Science in China Series B: Chemistry, 1997, 40, 657-662.	0.8	1
47	Theoretical study of dynamical properties on reaction path in molecular internal coordinates. Science in China Series B: Chemistry, 1999, 42, 605-611.	0.8	1
48	Structures, electronic properties, hydration and UV-vis absorption spectra of actinide motexafins [An-Motex]2+ (Anâ€‰=â€‰Ac, Cm, Lr) and [UO2-Motex]1+: insights from DFT calculations. Molecular Physics, 2020, 118, e1736676.	1.7	1