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	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
2	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
3	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
4	The Origin of the Photoluminescence Enhancement of Goldâ€Doped Silver Nanoclusters: The Importance of Relativistic Effects and Heteronuclear Goldâ€“Silver Bonds. Angewandte Chemie - International Edition, 2018, 57, 9965-9969.	13.8	53
5	Ursache der PhotolumineszenzverstÃ¤rkung in Goldâ€dotierten Silberâ€Nanoclustern: BeitrÃ¤ge relativistischer Effekte und heteronuklearer Goldâ€Silberâ€Bindungen. Angewandte Chemie, 2018, 130, 10114-10119.	2.0	6
6	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
7	Energy Resonance Crossing Controls the Photoluminescence of Europium Antenna Probes. Angewandte Chemie - International Edition, 2017, 56, 7986-7990.	13.8	23
8	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
9	Energieresonanzkreuzung steuert die Photolumineszenz von Europiumâ€Antennensonden. Angewandte Chemie, 2017, 129, 8097-8101.	2.0	4
10	Quantum chemical study of the autoxidation of ascorbate. Journal of Computational Chemistry, 2016, 37, 1914-1923.	3.3	4
11	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
12	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
13	Relativistic Small-Core Pseudopotentials for Actinium, Thorium, and Protactinium. Journal of Physical Chemistry A, 2014, 118, 2519-2530.	2.5	60
14	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
15	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
16	Relativistic Pseudopotentials: Their Development and Scope of Applications. Chemical Reviews, 2012, 112, 403-480.	47.7	346
17	Pseudopotentials and modelpotentials. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 200-210.	14.6	37
18	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

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19	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
20	Computational study of lanthanide(iii) hydration. Physical Chemistry Chemical Physics, 2010, 12, 13215.	2.8	96
21	Relativistic Pseudopotentials. Challenges and Advances in Computational Chemistry and Physics, 2010, , 215-277.	0.6	23
22	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
23	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
24	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
25	Approaching actinide(+III) hydration from first principles. Physical Chemistry Chemical Physics, 2007, 9, 459-465.	2.8	94
26	Quasirelativistic energy-consistent 5f-in-core pseudopotentials for trivalent actinide elements. Theoretical Chemistry Accounts, 2007, 117, 473-481.	1.4	88
27	Quasirelativistic energy-consistent 5f-in-core pseudopotentials for divalent and tetravalent actinide elements. Theoretical Chemistry Accounts, 2007, 118, 845-854.	1.4	78
28	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
29	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
30	Ab initio studies on the electronic structure of FeOH. Chemical Physics, 2005, 311, 203-208.	1.9	10
31	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
32	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
33	Segmented contraction scheme for small-core actinide pseudopotential basis sets. Computational and Theoretical Chemistry, 2004, 673, 203-209.	1.5	616
34	Electron affinity of Ce and electronic states ofCeâ^'. Physical Review A, 2004, 69, .	2.5	18
35	Valence basis sets for relativistic energy-consistent small-core actinide pseudopotentials. Journal of Chemical Physics, 2003, 118, 487-496.	3.0	640
36	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

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37	Theoretical prediction of the second to fourth actinide ionization potentials. Molecular Physics, 2003, 101, 961-969.	1.7	54
38	Electronic structure of lanthanide dimers. Molecular Physics, 2003, 101, 1967-1976.	1.7	44
39	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
40	Molecular structure of diatomic lanthanide compounds. Science in China Series B: Chemistry, 2002, 45, 91.	0.8	37
41	Pseudopotential study of lanthanum and lutetium dimers. Theoretical Chemistry Accounts, 2002, 108, 143-149.	1.4	43
42	Segmented contraction scheme for small-core lanthanide pseudopotential basis sets. Computational and Theoretical Chemistry, 2002, 581, 139-147.	1.5	653
43	Valence basis sets for relativistic energy-consistent small-core lanthanide pseudopotentials. Journal of Chemical Physics, 2001, 115, 7348-7355.	3.0	574
44	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
45	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
46	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
47	HeI photoelectron spectroscopic study of the electronic structure of SSF2 and FSSF compounds. Chemical Physics Letters, 1998, 290, 405-408.	2.6	9
48	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