

Lan Cheng

List of Publications by Year in descending order

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58
papers

1,787
citations

331670

21
h-index

276875

41
g-index

58
all docs

58
docs citations

58
times ranked

1476
citing authors

#	ARTICLE	IF	CITATIONS
1	Coupled-cluster techniques for computational chemistry: The <code>CFOUR</code> program package. <i>Journal of Chemical Physics</i> , 2020, 152, 214108.	3.0	375
2	Making four- and two-component relativistic density functional methods fully equivalent based on the idea of “from atoms to molecule”. <i>Journal of Chemical Physics</i> , 2007, 127, 104106.	3.0	210
3	Analytic energy gradients for the spin-free exact two-component theory using an exact block diagonalization for the one-electron Dirac Hamiltonian. <i>Journal of Chemical Physics</i> , 2011, 135, 084114.	3.0	136
4	The Simplest Criegee Intermediate (H_2CO_2): Isotopic Spectroscopy, Equilibrium Structure, and Possible Formation from Atmospheric Lightning. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 4133-4139.	4.6	88
5	Bond Dissociation Energies for Diatomic Molecules Containing 3d Transition Metals: Benchmark Scalar-Relativistic Coupled-Cluster Calculations for 20 Molecules. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1044-1056.	5.3	81
6	An atomic mean-field spin-orbit approach within exact two-component theory for a non-perturbative treatment of spin-orbit coupling. <i>Journal of Chemical Physics</i> , 2018, 148, 144108.	3.0	58
7	Benchmark Calculations of K-Edge Ionization Energies for First-Row Elements Using Scalar-Relativistic Core-Valence-Separated Equation-of-Motion Coupled-Cluster Methods. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1642-1651.	5.3	54
8	Performance of Delta-Coupled-Cluster Methods for Calculations of Core-Ionization Energies of First-Row Elements. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4945-4955.	5.3	50
9	Analytical evaluation of first-order electrical properties based on the spin-free Dirac-Coulomb Hamiltonian. <i>Journal of Chemical Physics</i> , 2011, 134, 244112.	3.0	42
10	Two-component relativistic coupled-cluster methods using mean-field spin-orbit integrals. <i>Journal of Chemical Physics</i> , 2018, 148, 034106.	3.0	42
11	Perturbative treatment of spin-orbit-coupling within spin-free exact two-component theory using equation-of-motion coupled-cluster methods. <i>Journal of Chemical Physics</i> , 2018, 148, 044108.	3.0	40
12	Analytic second derivatives for the spin-free exact two-component theory. <i>Journal of Chemical Physics</i> , 2011, 135, 244104.	3.0	35
13	Analytic energy derivatives in relativistic quantum chemistry. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 1108-1127.	2.0	35
14	Exact two-component equation-of-motion coupled-cluster singles and doubles method using atomic mean-field spin-orbit integrals. <i>Journal of Chemical Physics</i> , 2019, 150, 074102.	3.0	32
15	Accurate prediction and measurement of vibronic branching ratios for laser cooling linear polyatomic molecules. <i>Journal of Chemical Physics</i> , 2021, 155, 091101.	3.0	30
16	An analysis of the performance of coupled cluster methods for K-edge core excitations and ionizations using standard basis sets. <i>Advances in Quantum Chemistry</i> , 2019, 79, 241-261.	0.8	30
17	Perturbative treatment of spin-orbit coupling within spin-free exact two-component theory. <i>Journal of Chemical Physics</i> , 2014, 141, 164107.	3.0	27
18	A theoretical and experimental benchmark study of core-excited states in nitrogen. <i>Journal of Chemical Physics</i> , 2018, 148, 064106.	3.0	27

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19	Unitary coupled-cluster based self-consistent polarization propagator theory: A third-order formulation and pilot applications. <i>Journal of Chemical Physics</i> , 2018, 148, 244110.	3.0	27
20	Relativistic coupled-cluster and equation-of-motion coupled-cluster methods. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1536.	14.6	26
21	Rotational spectra of rare isotopic species of fluoroiodomethane: Determination of the equilibrium structure from rotational spectroscopy and quantum-chemical calculations. <i>Journal of Chemical Physics</i> , 2012, 137, 024310.	3.0	24
22	Coupled cluster study of the x-ray absorption spectra of formaldehyde derivatives at the oxygen, carbon, and fluorine K-edges. <i>Journal of Chemical Physics</i> , 2019, 151, 064107.	3.0	24
23	Branching Ratios, Radiative Lifetimes, and Transition Dipole Moments for YbOH. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3135-3148.	2.5	20
24	The route to high accuracy in <i>ab initio</i> calculations of Cu quadrupole-coupling constants. <i>Journal of Chemical Physics</i> , 2012, 137, 224302.	3.0	17
25	Matrix-Isolation and Quantum-Chemical Analysis of the C _{3v} Conformer of XeF ₆ , XeOF ₄ , and Their Acetonitrile Adducts. <i>Journal of Physical Chemistry A</i> , 2018, 122, 119-129.	2.5	17
26	Spin-free Dirac-Coulomb calculations augmented with a perturbative treatment of spin-orbit effects at the Hartree-Fock level. <i>Journal of Chemical Physics</i> , 2013, 139, 214114.	3.0	15
27	Inner-shell photoionization and core-hole decay of Xe and XeF ₂ . <i>Journal of Chemical Physics</i> , 2015, 142, 224302.	3.0	15
28	Low-lying vibronic level structure of the ground state of the methoxy radical: Slow electron velocity-map imaging (SEVI) spectra and K�ppel-Domcke-Cederbaum (KDC) vibronic Hamiltonian calculations. <i>Journal of Chemical Physics</i> , 2017, 146, 224309.	3.0	15
29	Performance of an atomic mean-field spin-orbit approach within exact two-component theory for perturbative treatment of spin-orbit coupling. <i>Molecular Physics</i> , 2020, 118, e1768313.	1.7	15
30	Atomic Mean-Field Approach within Exact Two-Component Theory Based on the Dirac-Coulomb-Breit Hamiltonian. <i>Journal of Physical Chemistry A</i> , 2022, 126, 4537-4553.	2.5	15
31	A study of non-iterative triples contributions in relativistic equation-of-motion coupled-cluster calculations using an exact two-component Hamiltonian with atomic mean-field spin-orbit integrals: Application to uranyl and other heavy-element compounds. <i>Journal of Chemical Physics</i> , 2019, 151, 104103.	3.0	14
32	Relativistic coupled-cluster calculations on XeF ₆ : Delicate interplay between electron-correlation and basis-set effects. <i>Journal of Chemical Physics</i> , 2015, 142, 224309.	3.0	13
33	Hetero-site Double Core Ionization Energies with Sub-electronvolt Accuracy from Delta-Coupled-Cluster Calculations. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4413-4426.	2.5	11
34	Analytic evaluation of energy first derivatives for spin-orbit coupled-cluster singles and doubles augmented with noniterative triples method: General formulation and an implementation for first-order properties. <i>Journal of Chemical Physics</i> , 2021, 154, 064110.	3.0	11
35	Direct perturbation theory in terms of energy derivatives: Scalar-relativistic treatment up to sixth order. <i>Journal of Chemical Physics</i> , 2011, 135, 194114.	3.0	10
36	Towards accurate prediction for laser-coolable molecules: relativistic coupled-cluster calculations for yttrium monoxide and prospects for improving its laser cooling efficiencies. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 26167-26177.	2.8	10

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37	Calculations of time-reversal-symmetry-violation sensitivity parameters based on analytic relativistic coupled-cluster gradient theory. <i>Physical Review A</i> , 2021, 104, .	2.5	10
38	Visible and ultraviolet laser spectroscopy of ThF. <i>Journal of Molecular Spectroscopy</i> , 2019, 358, 1-16.	1.2	8
39	Mapping the Electronic Structure of the Uranium(VI) Dinitride Molecule, UN ₂ . <i>Journal of Physical Chemistry A</i> , 2020, 124, 6486-6492.	2.5	8
40	Inner-shell excitation in the YbF molecule and its impact on laser cooling. <i>Journal of Molecular Spectroscopy</i> , 2022, 386, 111625.	1.2	8
41	The bromine nuclear quadrupole moment revisited. <i>Molecular Physics</i> , 2013, 111, 1382-1389.	1.7	7
42	The electric dipole moments in the ground states of gold oxide, AuO, and gold sulfide, AuS. <i>Journal of Chemical Physics</i> , 2017, 146, 064307.	3.0	7
43	Spectroscopy on the electron-electric-dipole-moment sensitive states of ThF^+ . <i>Physical Review A</i> , 2022, 105, .	2.5	7
44	Optical Stark and Zeeman Spectroscopy of Thorium Fluoride (ThF) and Thorium Chloride (ThCl). <i>Journal of Physical Chemistry A</i> , 2019, 123, 1423-1433.	2.5	6
45	Unitary coupled-cluster based self-consistent polarization propagator theory: A quadratic unitary coupled-cluster singles and doubles scheme. <i>Journal of Chemical Physics</i> , 2021, 155, 174102.	3.0	5
46	Geometry optimizations with spinor-based relativistic coupled-cluster theory. <i>Journal of Chemical Physics</i> , 2022, 156, 151101.	3.0	5
47	Electronic structure of NdO via slow photoelectron velocity-map imaging spectroscopy of NdO ⁺ . <i>Journal of Chemical Physics</i> , 2021, 155, 114305.	3.0	4
48	Quadratic Unitary Coupled-Cluster Singles and Doubles Scheme: Efficient Implementation, Benchmark Study, and Formulation of an Extended Version. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2281-2291.	5.3	4
49	The permanent electric dipole moment of gold chloride, AuCl. <i>Molecular Physics</i> , 2015, 113, 2073-2080.	1.7	3
50	Anion photoelectron spectroscopic and relativistic coupled-cluster studies of uranyl dichloride anion, UO_2Cl_2^- .	1.2	3
51	Multiphoton Control of 6 ϵ Photocyclization via State-Dependent Reactant-Product Correlations. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 9493-9500.	4.6	3
52	Photoelectron Spectroscopic and <i>ab Initio</i> Computational Studies of the Anion, HThO^+ .	2.5	2
53	Benchmark Relativistic Delta-Coupled-Cluster Calculations of K-Edge Core-Ionization Energies for Third-Row Elements. <i>Physical Chemistry Chemical Physics</i> , 0, , .	2.8	2
54	Photoelectron spectroscopy of cryogenically cooled NiO ₂ ⁺ via slow photoelectron velocity-map imaging. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 17496-17503.	2.8	2

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55	Benchmark calculations on the nuclear quadrupole-coupling parameters for open-shell molecules using non-relativistic and scalar-relativistic coupled-cluster methods. <i>Journal of Chemical Physics</i> , 2015, 143, 064301.	3.0	1
56	Limitations of perturbative coupled-cluster approximations for highly accurate investigations of Rb^{2+} . <i>Journal of Chemical Physics</i> , 2021, 155, 124101.	3.0	1
57	Characterization of the $[18.28]0\hat{a}^{\sim}a3^{\hat{1}}1$ (0,0) band of tantalum nitride, TaN. <i>Journal of Chemical Physics</i> , 2017, 147, 154304.	3.0	0
58	Introduction to the John Stanton special issue. <i>Molecular Physics</i> , 0, , .	1.7	0