Lan Cheng

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7739067/publications.pdf

Version: 2024-02-01

58 papers	1,787 citations	331538 21 h-index	276775 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 <scp>CFOUR</scp> program package. Journal of Chemical Physics, 2020, 152, 214108.	1.2	375
2	Making four- and two-component relativistic density functional methods fully equivalent based on the idea of â€œfrom atoms to moleculeâ€• Journal of Chemical Physics, 2007, 127, 104106.	1.2	210
3	Analytic energy gradients for the spin-free exact two-component theory using an exact block diagonalization for the one-electron Dirac Hamiltonian. Journal of Chemical Physics, 2011, 135, 084114.	1.2	136
4	The Simplest Criegee Intermediate (H₂Câ•Oâ€“O): Isotopic Spectroscopy, Equilibrium Structure, and Possible Formation from Atmospheric Lightning. Journal of Physical Chemistry Letters, 2013, 4, 4133-4139.	2.1	88
5	Bond Dissociation Energies for Diatomic Molecules Containing 3d Transition Metals: Benchmark Scalar-Relativistic Coupled-Cluster Calculations for 20 Molecules. Journal of Chemical Theory and Computation, 2017, 13, 1044-1056.	2.3	81
6	An atomic mean-field spin-orbit approach within exact two-component theory for a non-perturbative treatment of spin-orbit coupling. Journal of Chemical Physics, 2018, 148, 144108.	1.2	58
7	Benchmark Calculations of K-Edge Ionization Energies for First-Row Elements Using Scalar-Relativistic Coreâ€“Valence-Separated Equation-of-Motion Coupled-Cluster Methods. Journal of Chemical Theory and Computation, 2019, 15, 1642-1651.	2.3	54
8	Performance of Delta-Coupled-Cluster Methods for Calculations of Core-Ionization Energies of First-Row Elements. Journal of Chemical Theory and Computation, 2019, 15, 4945-4955.	2.3	50
9	Analytical evaluation of first-order electrical properties based on the spin-free Dirac-Coulomb Hamiltonian. Journal of Chemical Physics, 2011, 134, 244112.	1.2	42
10	Two-component relativistic coupled-cluster methods using mean-field spin-orbit integrals. Journal of Chemical Physics, 2018, 148, 034106.	1.2	42
11	Perturbative treatment of spin-orbit-coupling within spin-free exact two-component theory using equation-of-motion coupled-cluster methods. Journal of Chemical Physics, 2018, 148, 044108.	1.2	40
12	Analytic second derivatives for the spin-free exact two-component theory. Journal of Chemical Physics, 2011, 135, 244104.	1.2	35
13	Analytic energy derivatives in relativistic quantum chemistry. International Journal of Quantum Chemistry, 2014, 114, 1108-1127.	1.0	35
14	Exact two-component equation-of-motion coupled-cluster singles and doubles method using atomic mean-field spin-orbit integrals. Journal of Chemical Physics, 2019, 150, 074102.	1.2	32
15	Accurate prediction and measurement of vibronic branching ratios for laser cooling linear polyatomic molecules. Journal of Chemical Physics, 2021, 155, 091101.	1.2	30
16	An analysis of the performance of coupled cluster methods for K-edge core excitations and ionizations using standard basis sets. Advances in Quantum Chemistry, 2019, 79, 241-261.	0.4	30
17	Perturbative treatment of spin-orbit coupling within spin-free exact two-component theory. Journal of Chemical Physics, 2014, 141, 164107.	1.2	27
18	A theoretical and experimental benchmark study of core-excited states in nitrogen. Journal of Chemical Physics, 2018, 148, 064106.	1.2	27

#	Article	IF	Citations
19	Unitary coupled-cluster based self-consistent polarization propagator theory: A third-order formulation and pilot applications. Journal of Chemical Physics, 2018, 148, 244110.	1.2	27
20	Relativistic coupledâ€cluster and equationâ€ofâ€motion coupledâ€cluster methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1536.	6.2	26
21	Rotational spectra of rare isotopic species of fluoroiodomethane: Determination of the equilibrium structure from rotational spectroscopy and quantum-chemical calculations. Journal of Chemical Physics, 2012, 137, 024310.	1.2	24
22	Coupled cluster study of the x-ray absorption spectra of formaldehyde derivatives at the oxygen, carbon, and fluorine K-edges. Journal of Chemical Physics, 2019, 151, 064107.	1.2	24
23	Branching Ratios, Radiative Lifetimes, and Transition Dipole Moments for YbOH. Journal of Physical Chemistry A, 2020, 124, 3135-3148.	1.1	20
24	The route to high accuracy in ab initio calculations of Cu quadrupole-coupling constants. Journal of Chemical Physics, 2012, 137, 224302.	1.2	17
25	Matrix-Isolation and Quantum-Chemical Analysis of the C3v Conformer of XeF6, XeOF4, and Their Acetonitrile Adducts. Journal of Physical Chemistry A, 2018, 122, 119-129.	1.1	17
26	Spin-free Dirac-Coulomb calculations augmented with a perturbative treatment of spin-orbit effects at the Hartree-Fock level. Journal of Chemical Physics, 2013, 139, 214114.	1.2	15
27	Inner-shell photoionization and core-hole decay of Xe and XeF2. Journal of Chemical Physics, 2015, 142, 224302.	1.2	15
28	Low-lying vibronic level structure of the ground state of the methoxy radical: Slow electron velocity-map imaging (SEVI) spectra and KÃ¶ppel-Domcke-Cederbaum (KDC) vibronic Hamiltonian calculations. Journal of Chemical Physics, 2017, 146, 224309.	1.2	15
29	Performance of an atomic mean-field spinâ€“orbit approach within exact two-component theory for perturbative treatment of spinâ€“orbit coupling. Molecular Physics, 2020, 118, e1768313.	0.8	15
30	Atomic Mean-Field Approach within Exact Two-Component Theory Based on the Diracâ€“Coulombâ€“Breit Hamiltonian. Journal of Physical Chemistry A, 2022, 126, 4537-4553.	1.1	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. Journal of Chemical Physics, 2019, 151, 104103.	1.2	14
32	Relativistic coupled-cluster calculations on XeF6: Delicate interplay between electron-correlation and basis-set effects. Journal of Chemical Physics, 2015, 142, 224309.	1.2	13
33	Hetero-site Double Core Ionization Energies with Sub-electronvolt Accuracy from Delta-Coupled-Cluster Calculations. Journal of Physical Chemistry A, 2020, 124, 4413-4426.	1.1	11
34	Analytic evaluation of energy first derivatives for spinâ€“orbit coupled-cluster singles and doubles augmented with noniterative triples method: General formulation and an implementation for first-order properties. Journal of Chemical Physics, 2021, 154, 064110.	1.2	11
35	Direct perturbation theory in terms of energy derivatives: Scalar-relativistic treatment up to sixth order. Journal of Chemical Physics, 2011, 135, 194114.	1.2	10
36	Towards accurate prediction for laser-coolable molecules: relativistic coupled-cluster calculations for yttrium monoxide and prospects for improving its laser cooling efficiencies. Physical Chemistry Chemical Physics, 2020, 22, 26167-26177.	1.3	10

#	Article	IF	Citations
37	Calculations of time-reversal-symmetry-violation sensitivity parameters based on analytic relativistic coupled-cluster gradient theory. Physical Review A, 2021, 104, .	1.0	10
38	Visible and ultraviolet laser spectroscopy of ThF. Journal of Molecular Spectroscopy, 2019, 358, 1-16.	0.4	8
39	Mapping the Electronic Structure of the Uranium(VI) Dinitride Molecule, UN2. Journal of Physical Chemistry A, 2020, 124, 6486-6492.	1.1	8
40	Inner-shell excitation in the YbF molecule and its impact on laser cooling. Journal of Molecular Spectroscopy, 2022, 386, 111625.	0.4	8
41	The bromine nuclear quadrupole moment revisited. Molecular Physics, 2013, 111, 1382-1389.	0.8	7
42	The electric dipole moments in the ground states of gold oxide, AuO, and gold sulfide, AuS. Journal of Chemical Physics, 2017, 146, 064307.	1.2	7
43	Spectroscopy on the electron-electric-dipole-momentâ€“sensitive states of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mi mathvariant="normal">ThF</mml:mi><mml:mo>+</mml:mo></mml:msup></mml:math>. Physical Review A, 2022, 105, .	1.0	7
44	Optical Stark and Zeeman Spectroscopy of Thorium Fluoride (ThF) and Thorium Chloride (ThCl). Journal of Physical Chemistry A, 2019, 123, 1423-1433.	1.1	6
45	Unitary coupled-cluster based self-consistent polarization propagator theory: A quadratic unitary coupled-cluster singles and doubles scheme. Journal of Chemical Physics, 2021, 155, 174102.	1.2	5
46	Geometry optimizations with spinor-based relativistic coupled-cluster theory. Journal of Chemical Physics, 2022, 156, 151101.	1.2	5
47	Electronic structure of NdO via slow photoelectron velocity-map imaging spectroscopy of NdO---. Journal of Chemical Physics, 2021, 155, 114305.	1.2	4
48	Quadratic Unitary Coupled-Cluster Singles and Doubles Scheme: Efficient Implementation, Benchmark Study, and Formulation of an Extended Version. Journal of Chemical Theory and Computation, 2022, 18, 2281-2291.	2.3	4
49	The permanent electric dipole moment of gold chloride, AuCl. Molecular Physics, 2015, 113, 2073-2080.	0.8	3
50	Anion photoelectron spectroscopic and relativistic coupled-cluster studies of uranyl dichloride anion, UO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e792" altimg="si74.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:math>Cl<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e800" altimg="si76.svg"><mml:msubsup><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow><mml:	0.4	3
51	Multiphoton Control of 6ï€ Photocyclization via State-Dependent Reactantâ€“Product Correlations. Journal of Physical Chemistry Letters, 2021, 12, 9493-9500.	2.1	3
52	Photoelectron Spectroscopic and ab Initio Computational Studies of the Anion, HThO^{â€“}. Journal of Physical Chemistry A, 2021, 125, 1903-1909.	1.1	2
53	Benchmark Relativistic Delta-Coupled-Cluster Calculations of K-Edge Core-Ionization Energies for Third-Row Elements. Physical Chemistry Chemical Physics, 0, , .	1.3	2
54	Photoelectron spectroscopy of cryogenically cooled NiO₂^{â^’}via slow photoelectron velocity-map imaging. Physical Chemistry Chemical Physics, 2022, 24, 17496-17503.	1.3	2

#	Article	IF	Citations
55	Benchmark calculations on the nuclear quadrupole-coupling parameters for open-shell molecules using non-relativistic and scalar-relativistic coupled-cluster methods. Journal of Chemical Physics, 2015, 143, 064301.	1.2	1
56	Limitations of perturbative coupled-cluster approximations for highly accurate investigations of Rb2+. Journal of Chemical Physics, 2021, 155, 124101.	1.2	1
57	Characterization of the [18.28]0â^'â€“a3Î”1 (0,0) band of tantalum nitride, TaN. Journal of Chemical Physics, 2017, 147, 154304.	1.2	0
58	Introduction to the John Stanton special issue. Molecular Physics, 0, , .	0.8	0