

Christof Holzer

List of Publications by Year in descending order

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Version: 2024-02-01

31
papers

1,351
citations

471509

17
h-index

395702

33
g-index

36
all docs

36
docs citations

36
times ranked

1341
citing authors

#	ARTICLE	IF	CITATIONS
1	TURBOMOLE: Modular program suite for <i>ab initio</i> quantum-chemical and condensed-matter simulations. <i>Journal of Chemical Physics</i> , 2020, 152, 184107.	3.0	616
2	Accuracy Assessment of <i>GW</i> Starting Points for Calculating Molecular Excitation Energies Using the Bethe–Salpeter Formalism. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2127-2136.	5.3	74
3	Experimental and Theoretical Determination of Dissociation Energies of Dispersion-Dominated Aromatic Molecular Complexes. <i>Chemical Reviews</i> , 2016, 116, 5614-5641.	47.7	62
4	Ionized, electron-attached, and excited states of molecular systems with spin–orbit coupling: Two-component <i>GW</i> and Bethe–Salpeter implementations. <i>Journal of Chemical Physics</i> , 2019, 150, 204116.	3.0	48
5	An improved seminumerical Coulomb and exchange algorithm for properties and excited states in modern density functional theory. <i>Journal of Chemical Physics</i> , 2020, 153, 184115.	3.0	48
6	The furan microsolvation blind challenge for quantum chemical methods: First steps. <i>Journal of Chemical Physics</i> , 2018, 148, 014301.	3.0	44
7	18-Crown-6 Coordinated Metal Halides with Bright Luminescence and Nonlinear Optical Effects. <i>Journal of the American Chemical Society</i> , 2021, 143, 798-804.	13.7	44
8	Assessing the Accuracy of Local Hybrid Density Functional Approximations for Molecular Response Properties. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2928-2947.	5.3	39
9	Quasirelativistic two-component core excitations and polarisabilities from a damped-response formulation of the Bethe–Salpeter equation. <i>Molecular Physics</i> , 2020, 118, e1755064.	1.7	38
10	The first microsolvation step for furans: New experiments and benchmarking strategies. <i>Journal of Chemical Physics</i> , 2020, 152, 164303.	3.0	28
11	Communication: A hybrid Bethe–Salpeter/time-dependent density-functional-theory approach for excitation energies. <i>Journal of Chemical Physics</i> , 2018, 149, 101101.	3.0	27
12	Communication: Symmetry-adapted perturbation theory with intermolecular induction and dispersion energies from the Bethe–Salpeter equation. <i>Journal of Chemical Physics</i> , 2017, 147, 181101.	3.0	25
13	Bethe–Salpeter correlation energies of atoms and molecules. <i>Journal of Chemical Physics</i> , 2018, 149, 144106.	3.0	24
14	Boosting Light Emission from Single Hydrogen Phthalocyanine Molecules by Charging. <i>Nano Letters</i> , 2020, 20, 7600-7605.	9.1	24
15	<i>GW</i> quasiparticle energies of atoms in strong magnetic fields. <i>Journal of Chemical Physics</i> , 2019, 150, 214112.	3.0	21
16	Synthesis of New Donor–Substituted Biphenyls: Preligands for Highly Luminescent (C ⁺ C ^D) Gold(III) Pincer Complexes. <i>Chemistry - A European Journal</i> , 2020, 26, 17156-17164.	3.3	21
17	A local hybrid exchange functional approximation from first principles. <i>Journal of Chemical Physics</i> , 2022, 157, .	3.0	18
18	NMR Coupling Constants Based on the Bethe–Salpeter Equation in the <i>GW</i> Approximation. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1030-1045.	5.3	17

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19	Vibrational Coherence Controls Molecular Fragmentation: Ultrafast Photodynamics of the [Ag ₂ Cl] ⁺ Scaffold. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 804-810.	4.6	14
20	The GW/BSE Method in Magnetic Fields. <i>Frontiers in Chemistry</i> , 2021, 9, 746162.	3.6	14
21	Explicitly Correlated Dispersion and Exchange Dispersion Energies in Symmetry-Adapted Perturbation Theory. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5965-5986.	5.3	13
22	A Multi-Scale Approach for Modeling the Optical Response of Molecular Materials Inside Cavities. <i>Advanced Materials</i> , 2022, 34, e2200350.	21.0	13
23	Impact of the current density on paramagnetic NMR properties. <i>Journal of Chemical Physics</i> , 2022, 157, .	3.0	13
24	Quasi-relativistic two-component computations of intermolecular dispersion energies. <i>Molecular Physics</i> , 2017, 115, 2775-2781.	1.7	12
25	Linear Response of Current-Dependent Density Functional Approximations in Magnetic Fields. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 4335-4341.	4.6	11
26	Coordinative Flexibility of a Thiophenolate Oxazoline Ligand in Nickel(II), Palladium(II), and Platinum(II) Complexes. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 1569-1578.	2.0	8
27	Mercaptoaryl-Oxazoline Complexes of Palladium and Their High Activities as Catalysts for Suzuki-Miyaura Coupling Reactions in Water. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 568-575.	2.0	8
28	Efficient Calculation of Magnetic Circular Dichroism Spectra Using Spin-Noncollinear Linear-Response Time-Dependent Density Functional Theory in Finite Magnetic Fields. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3747-3758.	5.3	7
29	Modeling and measuring plasmonic excitations in hollow spherical gold nanoparticles. <i>Journal of Chemical Physics</i> , 2022, 156, 094103.	3.0	5
30	Multiscale Modeling of Broadband Perfect Absorbers Based on Gold Metallic Molecules. <i>ACS Omega</i> , 2022, 7, .	3.5	3
31	A tetranuclear nickel(II) heterocubane complex of a bidentate N,O-hydroxymethyl-oxazoline ligand. Synthesis, characterization, magnetic measurements and DFT investigations. <i>Journal of Coordination Chemistry</i> , 2016, 69, 433-446.	2.2	2