

Pierre-Francois Loos

List of Publications by Citations

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111
papers

2,274
citations

26
h-index

41
g-index

126
ext. papers

2,835
ext. citations

4.1
avg, IF

6.08
L-index

#	Paper	IF	Citations
111	A Mountaineering Strategy to Excited States: Highly Accurate Reference Energies and Benchmarks. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 4360-4379	6.4	145
110	Hybrid stochastic-deterministic calculation of the second-order perturbative contribution of multireference perturbation theory. <i>Journal of Chemical Physics</i> , 2017 , 147, 034101	3.9	83
109	Reference Energies for Double Excitations. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 1939-1956	6.4	78
108	Two electrons on a hypersphere: a quasiexactly solvable model. <i>Physical Review Letters</i> , 2009 , 103, 123004	7.4	76
107	A theoretical study of Ru(II) polypyridyl DNA intercalators structure and electronic absorption spectroscopy of [Ru(phen) ₂ (dppz)] ²⁺ and [Ru(tap) ₂ (dppz)] ²⁺ complexes intercalated in guanine-cytosine base pairs. <i>Journal of Inorganic Biochemistry</i> , 2010 , 104, 893-901	4.2	68
106	Selected configuration interaction dressed by perturbation. <i>Journal of Chemical Physics</i> , 2018 , 149, 064103	3.9	68
105	Quantum Package 2.0: An Open-Source Determinant-Driven Suite of Programs. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 3591-3609	6.4	65
104	A Mountaineering Strategy to Excited States: Highly Accurate Energies and Benchmarks for Medium Sized Molecules. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 1711-1741	6.4	63
103	The uniform electron gas. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2016 , 6, 410-429	4.2	60
102	The Quest for Highly Accurate Excitation Energies: A Computational Perspective. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 2374-2383	6.4	58
101	Ground state of two electrons on a sphere. <i>Physical Review A</i> , 2009 , 79,	2.6	52
100	Exact wave functions of two-electron quantum rings. <i>Physical Review Letters</i> , 2012 , 108, 083002	7.4	47
99	Deterministic Construction of Nodal Surfaces within Quantum Monte Carlo: The Case of FeS. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 1395-1402	6.4	43
98	Excitation energies from diffusion Monte Carlo using selected configuration interaction nodes. <i>Journal of Chemical Physics</i> , 2018 , 149, 034108	3.9	41
97	The Bethe-Salpeter Equation Formalism: From Physics to Chemistry. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 7371-7382	6.4	38
96	Excited states of spherium. <i>Molecular Physics</i> , 2010 , 108, 2527-2532	1.7	37
95	Important effects of neighbouring nucleotides on electron induced DNA single-strand breaks. <i>Chemical Physics Letters</i> , 2009 , 475, 120-123	2.5	35

94	Cross-Comparisons between Experiment, TD-DFT, CC, and ADC for Transition Energies. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 4581-4590	6.4	34
93	Correlation energy of two electrons in the high-density limit. <i>Journal of Chemical Physics</i> , 2009 , 131, 2411-2419	3.0	34
92	Theoretical 0-0 Energies with Chemical Accuracy. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 4646-4654	6.4	33
91	DFT and TD-DFT investigation of IR and UV spectra of solvated molecules: Comparison of two SCRF continuum models. <i>International Journal of Quantum Chemistry</i> , 2007 , 107, 574-585	2.1	33
90	Mountaineering Strategy to Excited States: Highly Accurate Energies and Benchmarks for Exotic Molecules and Radicals. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 3720-3736	6.4	29
89	A tale of two electrons: Correlation at high density. <i>Chemical Physics Letters</i> , 2010 , 500, 1-8	2.5	29
88	Benchmarking TD-DFT and Wave Function Methods for Oscillator Strengths and Excited-State Dipole Moments. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 1117-1132	6.4	27
87	Uniform electron gases. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	26
86	Uniform electron gases. I. Electrons on a ring. <i>Journal of Chemical Physics</i> , 2013 , 138, 164124	3.9	26
85	Invariance of the correlation energy at high density and large dimension in two-electron systems. <i>Physical Review Letters</i> , 2010 , 105, 113001	7.4	26
84	Chemically Accurate 0-0 Energies with Not-so-Accurate Excited State Geometries. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 2481-2491	6.4	25
83	Green Functions and Self-Consistency: Insights From the Spherium Model. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 3071-3082	6.4	25
82	Thinking outside the box: the uniform electron gas on a hypersphere. <i>Journal of Chemical Physics</i> , 2011 , 135, 214111	3.9	25
81	Hooke's law correlation in two-electron systems. <i>Physical Review A</i> , 2010 , 81,	2.6	24
80	Effect of ring strain on disulfide electron attachment. <i>Chemical Physics Letters</i> , 2008 , 458, 276-280	2.5	24
79	QUESTDB: A database of highly accurate excitation energies for the electronic structure community. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021 , 11, e1517	7.9	24
78	Unphysical Discontinuities in GW Methods. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 5220-5228	6.4	24
77	Core-ionized and core-excited states of macromolecules. <i>International Journal of Quantum Chemistry</i> , 2007 , 107, 2243-2252	2.1	23

76	Correlation energy of two electrons in a ball. <i>Journal of Chemical Physics</i> , 2010 , 132, 234111	3.9	22
75	Theoretical Investigation of the Geometries and UV-vis Spectra of Poly(L-glutamic acid) Featuring a Photochromic Azobenzene Side Chain. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 637-45	6.4	22
74	Frozen core orbitals as an alternative to specific frontier bond potential in hybrid Quantum Mechanics/Molecular Mechanics methods. <i>Chemical Physics Letters</i> , 2006 , 427, 236-240	2.5	22
73	Evaluating 00 Energies with Theoretical Tools: A Short Review. <i>ChemPhotoChem</i> , 2019 , 3, 684-696	3.3	21
72	Chemically accurate excitation energies with small basis sets. <i>Journal of Chemical Physics</i> , 2019 , 151, 144118	3.9	21
71	High-density correlation energy expansion of the one-dimensional uniform electron gas. <i>Journal of Chemical Physics</i> , 2013 , 138, 064108	3.9	19
70	Ground state of two electrons on concentric spheres. <i>Physical Review A</i> , 2010 , 81,	2.6	19
69	A Density-Based Basis-Set Correction for Wave Function Theory. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 2931-2937	6.4	18
68	Uniform electron gases. II. The generalized local density approximation in one dimension. <i>Journal of Chemical Physics</i> , 2014 , 140, 18A524	3.9	17
67	Correlation energy of the spin-polarized uniform electron gas at high density. <i>Physical Review B</i> , 2011 , 84,	3.3	17
66	A weight-dependent local correlation density-functional approximation for ensembles. <i>Journal of Chemical Physics</i> , 2020 , 152, 214101	3.9	16
65	Solvent effects on the asymmetric Diels-Alder reaction between cyclopentadiene and (E)-menthyl acrylate revisited with the three-layer hybrid local self-consistent field/molecular mechanics/self-consistent reaction field method. <i>Theoretical Chemistry Accounts</i> , 2004 , 112, 228	1.9	16
64	Density-Based Basis-Set Incompleteness Correction for Methods. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 1018-1028	6.4	15
63	Pros and Cons of the Bethe-Salpeter Formalism for Ground-State Energies. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 3536-3545	6.4	15
62	The performance of CIPSI on the ground state electronic energy of benzene. <i>Journal of Chemical Physics</i> , 2020 , 153, 176101	3.9	15
61	Nodal surfaces and interdimensional degeneracies. <i>Journal of Chemical Physics</i> , 2015 , 142, 214112	3.9	14
60	Generalized local-density approximation and one-dimensional finite uniform electron gases. <i>Physical Review A</i> , 2014 , 89,	2.6	14
59	Three- and four-electron integrals involving Gaussian geminals: Fundamental integrals, upper bounds, and recurrence relations. <i>Journal of Chemical Physics</i> , 2017 , 147, 024103	3.9	14

58	Exact energy of the spin-polarized two-dimensional electron gas at high density. <i>Physical Review B</i> , 2011 , 83,	3.3	14
57	Self-Consistent Strictly Localized Orbitals. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 1047-536.4	6.4	14
56	Reference Energies for Intramolecular Charge-Transfer Excitations. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 3666-3686	6.4	14
55	Is ADC(3) as Accurate as CC3 for Valence and Rydberg Transition Energies?. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 974-980	6.4	13
54	Huge Disulfide-Linkage'S Electron Capture Variation Induced by β Helix Orientation. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 1171-3	6.4	13
53	Weight dependence of local exchange-correlation functionals in ensemble density-functional theory: double excitations in two-electron systems. <i>Faraday Discussions</i> , 2020 , 224, 402-423	3.6	12
52	Dynamical correction to the Bethe-Salpeter equation beyond the plasmon-pole approximation. <i>Journal of Chemical Physics</i> , 2020 , 153, 114120	3.9	12
51	Exchange functionals based on finite uniform electron gases. <i>Journal of Chemical Physics</i> , 2017 , 146, 114108	3.9	11
50	Complex adiabatic connection: A hidden non-Hermitian path from ground to excited states. <i>Journal of Chemical Physics</i> , 2019 , 150, 041103	3.9	11
49	Influence of pseudopotentials on excitation energies from selected configuration interaction and diffusion Monte Carlo. <i>Results in Chemistry</i> , 2019 , 1, 100002	2.1	11
48	Analyzing the Selectivity and Successiveness of a Two-Electron Capture on a Multiply Disulfide-Linked Protein. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 1700-8	6.4	11
47	Factors governing electron capture by small disulfide loops in two-cysteine peptides. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 13661-9	3.4	11
46	A TD-DFT investigation of UV spectra of pyranonic dyes: A NCM vs PCM comparison. <i>Computational and Theoretical Chemistry</i> , 2007 , 808, 85-91		11
45	Chemistry in one dimension. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 3196-206	3.6	10
44	Many-Electron Integrals over Gaussian Basis Functions. I. Recurrence Relations for Three-Electron Integrals. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 1735-40	6.4	10
43	Intramolecular interactions and cis peptidic bonds. <i>Theoretical Chemistry Accounts</i> , 2007 , 118, 165-171	1.9	10
42	Natural occupation numbers in two-electron quantum rings. <i>Journal of Chemical Physics</i> , 2016 , 144, 054108	3.9	10
41	Excited States From State-Specific Orbital-Optimized Pair Coupled Cluster. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 4756-4768	6.4	10

40	Variational coupled cluster for ground and excited states. <i>Journal of Chemical Physics</i> , 2021 , 155, 104105,9	3.9	10
39	A basis-set error correction based on density-functional theory for strongly correlated molecular systems. <i>Journal of Chemical Physics</i> , 2020 , 152, 174104	3.9	9
38	Uniform electron gases. III. Low-density gases on three-dimensional spheres. <i>Journal of Chemical Physics</i> , 2015 , 143, 084114	3.9	9
37	Mountaineering Strategy to Excited States: Highly Accurate Oscillator Strengths and Dipole Moments of Small Molecules. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 416-438	6.4	9
36	Potential Energy Surfaces without Unphysical Discontinuities: The Coulomb Hole Plus Screened Exchange Approach. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 191-200	6.4	9
35	Capturing static and dynamic correlation with M\O-MP2 and M\O-CCSD . <i>Journal of Chemical Physics</i> , 2020 , 152, 014101	3.9	8
34	Correlation energy of anisotropic quantum dots. <i>Physical Review A</i> , 2011 , 84,	2.6	8
33	A Wigner molecule at extremely low densities: a numerically exact study 2019 , 1,		8
32	Dynamical kernels for optical excitations. <i>Journal of Chemical Physics</i> , 2020 , 153, 184105	3.9	8
31	Perturbation theory in the complex plane: exceptional points and where to find them. <i>Journal of Physics Condensed Matter</i> , 2021 , 33,	1.8	8
30	Understanding excitons using spherical geometry. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2012 , 376, 1997-2000	2.3	7
29	Harmonically trapped jellium. <i>Molecular Physics</i> , 2012 , 110, 2337-2342	1.7	7
28	Leading-order behavior of the correlation energy in the uniform electron gas. <i>International Journal of Quantum Chemistry</i> , 2012 , 112, 1712-1716	2.1	7
27	Toward a systematic improvement of the fixed-node approximation in diffusion Monte Carlo for solids-A case study in diamond. <i>Journal of Chemical Physics</i> , 2020 , 153, 184111	3.9	7
26	Communication: Three-electron coalescence points in two and three dimensions. <i>Journal of Chemical Physics</i> , 2015 , 143, 181101	3.9	6
25	Distribution of r_{12}^{-12} in quantum systems. <i>Molecular Physics</i> , 2013 , 111, 2414-2426	1.7	6
24	Electronic effects and ring strain influences on the electron uptake by selenium-containing bonds. <i>International Journal of Quantum Chemistry</i> , 2010 , 110, 513-523	2.1	6
23	Spin-Conserved and Spin-Flip Optical Excitations from the Bethe-Salpeter Equation Formalism. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 2852-2867	6.4	6

22	Molecular electronic structure in one-dimensional Coulomb systems. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 3987-3998	3.6	5
21	Parity-Time Symmetry in Hartree-Fock Theory. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 4374-4385	6.4	5
20	Symmetry-broken local-density approximation for one-dimensional systems. <i>Physical Review B</i> , 2016 , 93,	3.3	5
19	Distributed Gaussian orbitals for the description of electrons in an external potential. <i>Journal of Molecular Modeling</i> , 2018 , 24, 216	2	5
18	Basis functions for electronic structure calculations on spheres. <i>Journal of Chemical Physics</i> , 2014 , 141, 244102	3.9	5
17	Taming the fixed-node error in diffusion Monte Carlo via range separation. <i>Journal of Chemical Physics</i> , 2020 , 153, 174107	3.9	5
16	Accurate full configuration interaction correlation energy estimates for five- and six-membered rings. <i>Journal of Chemical Physics</i> , 2021 , 155, 134104	3.9	4
15	Recurrence Relations for Four-Electron Integrals Over Gaussian Basis Functions. <i>Advances in Quantum Chemistry</i> , 2018 , 147-165	1.4	3
14	Exact wave functions for concentric two-electron systems. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2014 , 378, 329-333	2.3	3
13	How accurate are EOM-CC4 vertical excitation energies?. <i>Journal of Chemical Physics</i> , 2021 , 154, 221103	3.9	3
12	Variations of the Hartree-Fock fractional-spin error for one electron. <i>Journal of Chemical Physics</i> , 2021 , 155, 054107	3.9	3
11	Excited-state Wigner crystals. <i>Journal of Chemical Physics</i> , 2017 , 146, 044114	3.9	2
10	New approaches to study excited states in density functional theory: general discussion. <i>Faraday Discussions</i> , 2020 , 224, 483-508	3.6	2
9	Static and dynamic Bethe-Salpeter equations in the T-matrix approximation.. <i>Journal of Chemical Physics</i> , 2022 , 156, 164101	3.9	2
8	Strong correlation in density functional theory: general discussion. <i>Faraday Discussions</i> , 2020 , 224, 373-386	3.6	1
7	Hierarchy Configuration Interaction: Combining Seniority Number and Excitation Degree.. <i>Journal of Physical Chemistry Letters</i> , 2022 , 4342-4349	6.4	1
6	A Mountaineering Strategy to Excited States: Highly Accurate Energies and Benchmarks for Bicyclic Systems. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 10174-10188	2.8	0
5	Challenges for large scale simulation: general discussion. <i>Faraday Discussions</i> , 2020 , 224, 309-332	3.6	0

- 4 Spin-adapted selected configuration interaction in a determinant basis. *Advances in Quantum Chemistry*, **2021**, 83, 65-81 1.4 ○
- 3 Iterative stochastic subspace self-consistent field method. *Journal of Molecular Modeling*, **2017**, 23, 173 2
- 2 Uniform electron gases **2012**, 121-129
- 1 Self-consistent electron-nucleus cusp correction for molecular orbitals. *Advances in Quantum Chemistry*, **2019**, 79, 113-132 1.4