Pierre-Francois Loos

List of Publications by Year in Descending Order

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	Static and dynamic Bethe-Salpeter equations in the T-matrix approximation.. *Journal of Chemical Physics*, **2022**, 156, 164101	3.9	2
110	Hierarchy Configuration Interaction: Combining Seniority Number and Excitation Degree.. *Journal of Physical Chemistry Letters*, **2022**, 4342-4349	6.4	1
109	A Mountaineering Strategy to Excited States: Highly Accurate Energies and Benchmarks for Bicyclic Systems. *Journal of Physical Chemistry A*, **2021**, 125, 10174-10188	2.8	0
108	Spin-Conserved and Spin-Flip Optical Excitations from the Bethe-Salpeter Equation Formalism. *Journal of Chemical Theory and Computation*, **2021**, 17, 2852-2867	6.4	6
107	Reference Energies for Intramolecular Charge-Transfer Excitations. *Journal of Chemical Theory and Computation*, **2021**, 17, 3666-3686	6.4	14
106	How accurate are EOM-CC4 vertical excitation energies?. *Journal of Chemical Physics*, **2021**, 154, 221103	3.9	3
105	Perturbation theory in the complex plane: exceptional points and where to find them. *Journal of Physics Condensed Matter*, **2021**, 33,	1.8	8
104	Mountaineering Strategy to Excited States: Highly Accurate Oscillator Strengths and Dipole Moments of Small Molecules. *Journal of Chemical Theory and Computation*, **2021**, 17, 416-438	6.4	9
103	Potential Energy Surfaces without Unphysical Discontinuities: The Coulomb Hole Plus Screened Exchange Approach. *Journal of Chemical Theory and Computation*, **2021**, 17, 191-200	6.4	9
102	Spin-adapted selected configuration interaction in a determinant basis. *Advances in Quantum Chemistry*, **2021**, 83, 65-81	1.4	0
101	QUESTDB: A database of highly accurate excitation energies for the electronic structure community. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1517	7.9	24
100	Excited States from State-Specific Orbital-Optimized Pair Coupled Cluster. *Journal of Chemical Theory and Computation*, **2021**, 17, 4756-4768	6.4	10
99	Variations of the Hartree-Fock fractional-spin error for one electron. *Journal of Chemical Physics*, **2021**, 155, 054107	3.9	3
98	Variational coupled cluster for ground and excited states. *Journal of Chemical Physics*, **2021**, 155, 104105	3.9	10
97	Accurate full configuration interaction correlation energy estimates for five- and six-membered rings. *Journal of Chemical Physics*, **2021**, 155, 134104	3.9	4
96	Benchmarking TD-DFT and Wave Function Methods for Oscillator Strengths and Excited-State Dipole Moments. *Journal of Chemical Theory and Computation*, **2021**, 17, 1117-1132	6.4	27
95	A basis-set error correction based on density-functional theory for strongly correlated molecular systems. *Journal of Chemical Physics*, **2020**, 152, 174104	3.9	9

94	Mountaineering Strategy to Excited States: Highly Accurate Energies and Benchmarks for Exotic Molecules and Radicals. *Journal of Chemical Theory and Computation*, **2020**, 16, 3720-3736	6.4	29
93	Weight dependence of local exchange-correlation functionals in ensemble density-functional theory: double excitations in two-electron systems. *Faraday Discussions*, **2020**, 224, 402-423	3.6	12
92	A weight-dependent local correlation density-functional approximation for ensembles. *Journal of Chemical Physics*, **2020**, 152, 214101	3.9	16
91	The Quest for Highly Accurate Excitation Energies: A Computational Perspective. *Journal of Physical Chemistry Letters*, **2020**, 11, 2374-2383	6.4	58
90	Density-Based Basis-Set Incompleteness Correction for Methods. *Journal of Chemical Theory and Computation*, **2020**, 16, 1018-1028	6.4	15
89	Is ADC(3) as Accurate as CC3 for Valence and Rydberg Transition Energies?. *Journal of Physical Chemistry Letters*, **2020**, 11, 974-980	6.4	13
88	Capturing static and dynamic correlation with ℕO-MP2 and ℕO-CCSD. *Journal of Chemical Physics* , **2020**, 152, 014101	3.9	8
87	A Mountaineering Strategy to Excited States: Highly Accurate Energies and Benchmarks for Medium Sized Molecules. *Journal of Chemical Theory and Computation*, **2020**, 16, 1711-1741	6.4	63
86	Pros and Cons of the Bethe-Salpeter Formalism for Ground-State Energies. *Journal of Physical Chemistry Letters*, **2020**, 11, 3536-3545	6.4	15
85	Toward a systematic improvement of the fixed-node approximation in diffusion Monte Carlo for solids-A case study in diamond. *Journal of Chemical Physics*, **2020**, 153, 184111	3.9	7
84	Taming the fixed-node error in diffusion Monte Carlo via range separation. *Journal of Chemical Physics*, **2020**, 153, 174107	3.9	5
83	Dynamical kernels for optical excitations. *Journal of Chemical Physics*, **2020**, 153, 184105	3.9	8
82	Dynamical correction to the Bethe-Salpeter equation beyond the plasmon-pole approximation. *Journal of Chemical Physics*, **2020**, 153, 114120	3.9	12
81	The performance of CIPSI on the ground state electronic energy of benzene. *Journal of Chemical Physics*, **2020**, 153, 176101	3.9	15
80	Challenges for large scale simulation: general discussion. *Faraday Discussions*, **2020**, 224, 309-332	3.6	0
79	Strong correlation in density functional theory: general discussion. *Faraday Discussions*, **2020**, 224, 373-381	3.6	1
78	New approaches to study excited states in density functional theory: general discussion. *Faraday Discussions*, **2020**, 224, 483-508	3.6	2
77	The Bethe-Salpeter Equation Formalism: From Physics to Chemistry. *Journal of Physical Chemistry Letters*, **2020**, 11, 7371-7382	6.4	38

76	Reference Energies for Double Excitations. *Journal of Chemical Theory and Computation*, **2019**, 15, 1939-1956	6.4	78
75	Complex adiabatic connection: A hidden non-Hermitian path from ground to excited states. *Journal of Chemical Physics*, **2019**, 150, 041103	3.9	11
74	Parity-Time Symmetry in Hartree-Fock Theory. *Journal of Chemical Theory and Computation*, **2019**, 15, 4374-4385	6.4	5
73	A Density-Based Basis-Set Correction for Wave Function Theory. *Journal of Physical Chemistry Letters*, **2019**, 10, 2931-2937	6.4	18
72	Quantum Package 2.0: An Open-Source Determinant-Driven Suite of Programs. *Journal of Chemical Theory and Computation*, **2019**, 15, 3591-3609	6.4	65
71	Evaluating 0–0 Energies with Theoretical Tools: A Short Review. *ChemPhotoChem*, **2019**, 3, 684-696	3.3	21
70	Chemically Accurate 0-0 Energies with Not-so-Accurate Excited State Geometries. *Journal of Chemical Theory and Computation*, **2019**, 15, 2481-2491	6.4	25
69	Influence of pseudopotentials on excitation energies from selected configuration interaction and diffusion Monte Carlo. *Results in Chemistry*, **2019**, 1, 100002	2.1	11
68	Cross-Comparisons between Experiment, TD-DFT, CC, and ADC for Transition Energies. *Journal of Chemical Theory and Computation*, **2019**, 15, 4581-4590	6.4	34
67	Chemically accurate excitation energies with small basis sets. *Journal of Chemical Physics*, **2019**, 151, 144118	3.9	21
66	A Wigner molecule at extremely low densities: a numerically exact study **2019**, 1,		8
65	Self-consistent electron–nucleus cusp correction for molecular orbitals. *Advances in Quantum Chemistry*, **2019**, 79, 113-132	1.4	
64	Deterministic Construction of Nodal Surfaces within Quantum Monte Carlo: The Case of FeS. *Journal of Chemical Theory and Computation*, **2018**, 14, 1395-1402	6.4	43
63	Theoretical 0-0 Energies with Chemical Accuracy. *Journal of Physical Chemistry Letters*, **2018**, 9, 4646-4651	6.4	33
62	Excitation energies from diffusion Monte Carlo using selected configuration interaction nodes. *Journal of Chemical Physics*, **2018**, 149, 034108	3.9	41
61	Distributed Gaussian orbitals for the description of electrons in an external potential. *Journal of Molecular Modeling*, **2018**, 24, 216	2	5
60	Green Functions and Self-Consistency: Insights From the Spherium Model. *Journal of Chemical Theory and Computation*, **2018**, 14, 3071-3082	6.4	25
59	Recurrence Relations for Four-Electron Integrals Over Gaussian Basis Functions. *Advances in Quantum Chemistry*, **2018**, 147-165	1.4	3

58	Unphysical Discontinuities in GW Methods. *Journal of Chemical Theory and Computation*, **2018**, 14, 5220-5228	5.4	24
57	Selected configuration interaction dressed by perturbation. *Journal of Chemical Physics*, **2018**, 149, 064103	3.9	68
56	A Mountaineering Strategy to Excited States: Highly Accurate Reference Energies and Benchmarks. *Journal of Chemical Theory and Computation*, **2018**, 14, 4360-4379	6.4	145
55	Molecular electronic structure in one-dimensional Coulomb systems. *Physical Chemistry Chemical Physics*, **2017**, 19, 3987-3998	3.6	5
54	Excited-state Wigner crystals. *Journal of Chemical Physics*, **2017**, 146, 044114	3.9	2
53	Exchange functionals based on finite uniform electron gases. *Journal of Chemical Physics*, **2017**, 146, 114108	3.9	11
52	Hybrid stochastic-deterministic calculation of the second-order perturbative contribution of multireference perturbation theory. *Journal of Chemical Physics*, **2017**, 147, 034101	3.9	83
51	Three- and four-electron integrals involving Gaussian geminals: Fundamental integrals, upper bounds, and recurrence relations. *Journal of Chemical Physics*, **2017**, 147, 024103	3.9	14
50	Iterative stochastic subspace self-consistent field method. *Journal of Molecular Modeling*, **2017**, 23, 173	2	
49	Symmetry-broken local-density approximation for one-dimensional systems. *Physical Review B*, **2016**, 93,	3.3	5
48	The uniform electron gas. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2016**, 6, 410-429	7.9	60
47	Many-Electron Integrals over Gaussian Basis Functions. I. Recurrence Relations for Three-Electron Integrals. *Journal of Chemical Theory and Computation*, **2016**, 12, 1735-40	6.4	10
46	Natural occupation numbers in two-electron quantum rings. *Journal of Chemical Physics*, **2016**, 144, 054108	3.9	10
45	Nodal surfaces and interdimensional degeneracies. *Journal of Chemical Physics*, **2015**, 142, 214112	3.9	14
44	Chemistry in one dimension. *Physical Chemistry Chemical Physics*, **2015**, 17, 3196-206	3.6	10
43	Communication: Three-electron coalescence points in two and three dimensions. *Journal of Chemical Physics*, **2015**, 143, 181101	3.9	6
42	Uniform electron gases. III. Low-density gases on three-dimensional spheres. *Journal of Chemical Physics*, **2015**, 143, 084114	3.9	9
41	Exact wave functions for concentric two-electron systems. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2014**, 378, 329-333	2.3	3

40	Generalized local-density approximation and one-dimensional finite uniform electron gases. *Physical Review A*, **2014**, 89,	2.6	14
39	Basis functions for electronic structure calculations on spheres. *Journal of Chemical Physics*, **2014**, 141, 244102	3.9	5
38	Uniform electron gases. II. The generalized local density approximation in one dimension. *Journal of Chemical Physics*, **2014**, 140, 18A524	3.9	17
37	High-density correlation energy expansion of the one-dimensional uniform electron gas. *Journal of Chemical Physics*, **2013**, 138, 064108	3.9	19
36	Uniform electron gases. I. Electrons on a ring. *Journal of Chemical Physics*, **2013**, 138, 164124	3.9	26
35	Distribution of r12 p12 in quantum systems. *Molecular Physics*, **2013**, 111, 2414-2426	1.7	6
34	Understanding excitons using spherical geometry. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2012**, 376, 1997-2000	2.3	7
33	Uniform electron gases. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	26
32	Harmonically trapped jellium. *Molecular Physics*, **2012**, 110, 2337-2342	1.7	7
31	Leading-order behavior of the correlation energy in the uniform electron gas. *International Journal of Quantum Chemistry*, **2012**, 112, 1712-1716	2.1	7
30	Exact wave functions of two-electron quantum rings. *Physical Review Letters*, **2012**, 108, 083002	7.4	47
29	Uniform electron gases **2012**, 121-129		
28	Thinking outside the box: the uniform electron gas on a hypersphere. *Journal of Chemical Physics*, **2011**, 135, 214111	3.9	25
27	Correlation energy of anisotropic quantum dots. *Physical Review A*, **2011**, 84,	2.6	8
26	Exact energy of the spin-polarized two-dimensional electron gas at high density. *Physical Review B*, **2011**, 83,	3.3	14
25	Correlation energy of the spin-polarized uniform electron gas at high density. *Physical Review B*, **2011**, 84,	3.3	17
24	Invariance of the correlation energy at high density and large dimension in two-electron systems. *Physical Review Letters*, **2010**, 105, 113001	7.4	26
23	Hooke law correlation in two-electron systems. *Physical Review A*, **2010**, 81,	2.6	24

22	Ground state of two electrons on concentric spheres. *Physical Review A*, **2010**, 81,	2.6	19
21	Correlation energy of two electrons in a ball. *Journal of Chemical Physics*, **2010**, 132, 234111	3.9	22
20	Excited states of spherium. *Molecular Physics*, **2010**, 108, 2527-2532	1.7	37
19	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. *Journal of Inorganic Biochemistry*, **2010**, 104, 893-901	4.2	68
18	A tale of two electrons: Correlation at high density. *Chemical Physics Letters*, **2010**, 500, 1-8	2.5	29
17	Electronic effects and ring strain influences on the electron uptake by selenium-containing bonds. *International Journal of Quantum Chemistry*, **2010**, 110, 513-523	2.1	6
16	Important effects of neighbouring nucleotides on electron induced DNA single-strand breaks. *Chemical Physics Letters*, **2009**, 475, 120-123	2.5	35
15	Analyzing the Selectivity and Successiveness of a Two-Electron Capture on a Multiply Disulfide-Linked Protein. *Journal of Chemical Theory and Computation*, **2009**, 5, 1700-8	6.4	11
14	Ground state of two electrons on a sphere. *Physical Review A*, **2009**, 79,	2.6	52
13	Two electrons on a hypersphere: a quasiexactly solvable model. *Physical Review Letters*, **2009**, 103, 123008	7.4	76
12	Correlation energy of two electrons in the high-density limit. *Journal of Chemical Physics*, **2009**, 131, 241101	3.9	34
11	Huge Disulfide-Linkage'S Electron Capture Variation Induced by Helix Orientation. *Journal of Chemical Theory and Computation*, **2008**, 4, 1171-3	6.4	13
10	Theoretical Investigation of the Geometries and UV-vis Spectra of Poly(l-glutamic acid) Featuring a Photochromic Azobenzene Side Chain. *Journal of Chemical Theory and Computation*, **2008**, 4, 637-45	6.4	22
9	Factors governing electron capture by small disulfide loops in two-cysteine peptides. *Journal of Physical Chemistry B*, **2008**, 112, 13661-9	3.4	11
8	Effect of ring strain on disulfide electron attachment. *Chemical Physics Letters*, **2008**, 458, 276-280	2.5	24
7	Self-Consistent Strictly Localized Orbitals. *Journal of Chemical Theory and Computation*, **2007**, 3, 1047-53	6.4	14
6	A TD-DFT investigation of UV spectra of pyranoidic dyes: A NCM vs PCM comparison. *Computational and Theoretical Chemistry*, **2007**, 808, 85-91		11
5	DFT and TD-DFT investigation of IR and UV spectra of solvated molecules: Comparison of two SCRF continuum models. *International Journal of Quantum Chemistry*, **2007**, 107, 574-585	2.1	33

4	Core-ionized and core-excited states of macromolecules. *International Journal of Quantum Chemistry*, **2007**, 107, 2243-2252	2.1	23
3	Intramolecular interactions and cis peptidic bonds. *Theoretical Chemistry Accounts*, **2007**, 118, 165-171	1.9	10
2	Frozen core orbitals as an alternative to specific frontier bond potential in hybrid Quantum Mechanics/Molecular Mechanics methods. *Chemical Physics Letters*, **2006**, 427, 236-240	2.5	22
1	Solvent effects on the asymmetric Diels–Alder reaction between cyclopentadiene and (−)-menthyl acrylate revisited with the three-layer hybrid local self-consistent field/molecular mechanics/self-consistent reaction field method. *Theoretical Chemistry Accounts*, **2004**, 112, 228	1.9	16