

Publications

Pierre-François Loos

79. Capturing static and dynamic correlation with Δ NO-MP2 and Δ NO-CCSD,
J. W. Hollett and **P. F. Loos**,
J. Chem. Phys. (submitted)
78. Wigner localization at extremely low densities: a numerically exact ab initio study,
M. E. Azor, L. Brooke, S. Evangelisti, T. Leininger, **P. F. Loos**, N. Suaud, and J. A. Berger,
SciPost Phys. (submitted).
77. Chemically accurate excitation energies with small basis sets,
E. Giner, A. Scemama, J. Toulouse, and **P. F. Loos***,
J. Chem. Phys. (submitted)
76. Cross comparisons between experiment, TD-DFT, CC and ADC for transition energies,
C. Suellen, R. Garcia Freitas, **P. F. Loos**, and D. Jacquemin,
J. Chem. Theory Comput., **2019**, 15, 4581.
75. A density-based basis-set correction for wave function theory,
P. F. Loos*, B. Pradines, A. Scemama, J. Toulouse, and E. Giner,
J. Phys. Chem. Lett., **2019**, 10, 2931.
74. Influence of pseudopotentials on excitation energies from selected configuration interaction and diffusion Monte Carlo,
A. Scemama, M. Caffarel, A. Benali, D. Jacquemin and **P. F. Loos***,
Res. Chem., **2019**, 1, 100002.
73. \mathcal{PT} -symmetry in Hartree–Fock theory,
H. G. A. Burton, A. J. W. Thom and **P. F. Loos***,
J. Chem. Theory Comput., **2019**, 15, 4374.
72. Evaluating 0-0 energies with theoretical tools: a short review,
P. F. Loos and D. Jacquemin,
ChemPhotoChem, **2019**, 3, 684.
71. Quantum Package 2.0: an open-source determinant-driven suite of programs,
Y. Garniron, K. Gasperich, T. Applencourt, A. Benali, A. Ferté, J. Paquier, B. Pradines, R. Assaraf,
P. Reinhardt, J. Toulouse, P. Barbaresco, N. Renon, G. David, J. P. Malrieu, M. Véril, M. Caffarel, **P. F. Loos***, E. Giner and A. Scemama,
J. Chem. Theory Comput., **2019**, 15, 3591.
70. Self-consistent electron-nucleus cusp correction for molecular orbitals,
P. F. Loos*, A. Scemama and M. Caffarel,
Adv. Quantum Chem., (in press) arXiv:1902.03406

69. Chemically accurate 0-0 energies with not-so-accurate excited state geometries,
P. F. Loos and D. Jacquemin,
J. Chem. Theory Comput., **2019**, *15*, 2481.
68. Reference energies for double excitations,
P. F. Loos*, M. Boggio-Pasqua, A. Scemama, M. Caffarel and D. Jacquemin,
J. Chem. Theory Comput., **2019**, *15*, 1939.
67. Complex adiabatic connection: a hidden non-hermitian path from ground to excited states,
H. G. A. Burton, A. J. W. Thom and **P. F. Loos**,
J. Chem. Phys., **2019**, *150*, 041103.
66. Unphysical discontinuities in GW methods,
M. V  ril, P. Romaniello, J. A. Berger and **P. F. Loos***,
J. Chem. Theory Comput., **2018**, *14*, 5220.
65. Theoretical 0-0 energies with chemical accuracy,
P. F. Loos, N. Galland and D. Jacquemin,
J. Phys. Chem. Lett., **2018**, *9*, 4646.
64. Selected configuration interaction with dressed perturbation,
Y. Garniron, A. Scemama, E. Giner, M. Caffarel and **P. F. Loos***,
J. Chem. Phys., **2018**, *149*, 064103.
63. Excitation energies from diffusion Monte Carlo using selected configuration interaction nodes,
A. Scemama, A. Benali, D. Jacquemin, M. Caffarel and **P. F. Loos***,
J. Chem. Phys., **2018**, *149*, 034108.
62. A mountaineering strategy to excited states: highly-accurate reference energies and benchmarks,
P. F. Loos*, A. Scemama, A. Blondel, Y. Garniron, M. Caffarel and D. Jacquemin,
J. Chem. Theory Comput., **2018**, *14*, 4360.
61. Distributed gaussian orbitals for the description of electrons in an external potential,
L. Brooke, A. Diaz-Marquez, S. Evangelisti, T. Leininger, **P. F. Loos**, N. Suaud and J. A. Berger,
J. Mod. Mol., **2018**, (in press).
60. Green functions and self-consistency: insights from the spherium model,
P. F. Loos*, P. Romaniello and J. A. Berger,
J. Chem. Theory Comput., **2018**, *14*, 3071.
59. Deterministic construction of nodal surfaces within quantum Monte Carlo: the case of FeS,
A. Scemama, Y. Garniron, M. Caffarel and **P. F. Loos***,
J. Chem. Theory Comput., **2018**, *14*, 1395.
58. Recurrence relations for four-electron integrals over Gaussian basis functions,
G. M. J. Barca and **P. F. Loos***,
Adv. Quantum Chem., **2018**, *76*, 147.
57. Hybrid stochastic-deterministic calculation of the second-order perturbative contribution of
multireference perturbation theory,
Y. Garniron, A. Scemama, **P. F. Loos** and M. Caffarel,
J. Chem. Phys., **2017**, *147*, 034101.

56. Three-electron and four-electron integrals involving Gaussian geminals: fundamental integrals, upper bounds and recurrence relations,
G. M. J. Barca and **P. F. Loos***,
J. Chem. Phys., **2017**, *147*, 024103.
55. Iterative stochastic subspace self-consistent field method,
P. F. Loos*, J.-L. Rivail and X. Assfeld,
J. Mod. Mol., **2017**, *23*, 173.
54. Exchange functionals based on finite uniform electron gases,
P. F. Loos*, *J. Chem. Phys.*, **2017**, *146*, 114108.
53. Excited-state Wigner crystals,
F. J. M. Rogers and **P. F. Loos***,
J. Chem. Phys., **2017**, *146*, 044114.
52. Electronic structure calculations in one dimension,
C. J. Ball, **P. F. Loos** and P. M. W. Gill,
Phys. Chem. Chem. Phys., **2017**, *19*, 3987.
51. Symmetry-broken local-density approximation for one-dimensional systems,
F. J. M. Rogers, C. J. Ball and **P. F. Loos***,
Phys. Rev. B, **2016**, *93*, 235114.
50. The uniform electron gas,
P. F. Loos* and P. M. W. Gill,
WIREs Comput. Mol. Sci., **2016**, *6*, 410.
49. Many-electron integrals over Gaussian basis functions. I. Recurrence relations for three-electron integrals,
G. M. J. Barca, **P. F. Loos** and P. M. W. Gill,
J. Chem. Theory Comput., **2016**, *12*, 1735.
48. Natural occupation numbers in two-electron quantum rings,
V. Tognetti and **P. F. Loos**,
J. Chem. Phys., **2016**, *144*, 054108.
47. Three-electron coalescence points in two and three dimensions,
P. F. Loos*, N. J. Bloomfield and P. M. W. Gill,
J. Chem. Phys., **2015**, *143*, 181101.
46. Uniform electron gases: III. Low-density gases on three-dimensional spheres,
D. Agboola, A. L. Knol, P. M. W. Gill and **P. F. Loos***,
J. Chem. Phys., **2015**, *143*, 084114.
45. Nodal surfaces and interdimensional degeneracies,
P. F. Loos* and D. Bressanini,
J. Chem. Phys., **2015**, *142*, 214112.
44. Chemistry in one dimension,
P. F. Loos*, C. J. Ball and P. M. W. Gill,
Phys. Chem. Chem. Phys., **2015**, *17*, 3196.

43. Basis functions for electronic structure calculations on spheres,
P. M. W. Gill, **P. F. Loos** and D. Agboola,
J. Chem. Phys., **2014**, *141*, 244102.
42. Generalized local-density approximation and one-dimensional uniform electron gases,
P. F. Loos*, *Phys. Rev. A*, **2014**, *89*, 052523.
41. Uniform electron gases. II. The generalized local density approximation in one dimension,
P. F. Loos*, C. J. Ball and P. M. W. Gill,
J. Chem. Phys., **2014**, *140*, 18A524.
40. Exact wave functions for concentric two-electron systems,
P. F. Loos and P. M. W. Gill,
Phys. Lett. A, **2014**, *378*, 329.
39. Distribution of $r_{12} \cdot p_{12}$ in quantum systems,
Y. A. Bernard, **P. F. Loos** and P. M. W. Gill,
Mol. Phys., **2013**, *111*, 2414.
38. Uniform electron gases. II. Electrons on a ring,
P. F. Loos* and P. M. W. Gill,
J. Chem. Phys., **2013**, *138*, 164124.
37. High-density correlation energy expansion of the one-dimensional uniform electron gas,
P. F. Loos*,
J. Chem. Phys., **2013**, *138*, 064108.
36. Understanding excitons using spherical geometry,
P. F. Loos*,
Phys. Lett. A, **2012**, *376*, 1997.
35. Harmonically trapped jellium model,
P. F. Loos and P. M. W. Gill,
Mol. Phys., **2012**, *108*, 083002.
34. Exact wave functions of two-electron quantum rings,
P. F. Loos and P. M. W. Gill,
Phys. Rev. Lett., **2012**, *110*, 2337.
33. Leading-order behavior of the correlation energy in the uniform electron gas,
P. F. Loos and P. M. W. Gill,
Int. J. Quantum Chem., **2012**, *112*, 1712.
32. Uniform electron gases,
P. M. W. Gill and **P. F. Loos**,
Theor. Chem. Acc., **2012**, *131*, 1069.
31. Thinking outside the box: the uniform electron gas on a hypersphere,
P. F. Loos* and P. M. W. Gill,
J. Chem. Phys., **2011**, *135*, 214111.
30. Correlation energy of anisotropic quantum dots,
Y. Zhao, **P. F. Loos*** and P. M. W. Gill,
Phys. Rev. A, **2011**, *84*, 032513.

29. Correlation energy of the spin-polarized uniform electron gas at high density,
P. F. Loos and P. M. W. Gill,
Phys. Rev. B, **2011**, *84*, 033103.
28. Exact energy of the spin-polarized two-dimensional electron gas at high density,
P. F. Loos and P. M. W. Gill,
Phys. Rev. B, **2011**, *83*, 233102.
27. A tale of two electrons: correlation at high density,
P. F. Loos* and P. M. W. Gill,
Chem. Phys. Lett., **2010**, *500*, 1.
26. Invariance of the correlation energy at high density and large dimension for two-electron systems,
P. F. Loos and P. M. W. Gill,
Phys. Rev. Lett., **2010**, *105*, 113001.
25. Excited states of spherium,
P. F. Loos and P. M. W. Gill,
Mol. Phys., **2010**, *108*, 2527.
24. Correlation energy of two electrons in a ball,
P. F. Loos* and P. M. W. Gill,
J. Chem. Phys., **2010**, *132*, 234111.
23. Ground state of two electrons on concentric spheres,
P. F. Loos and P. M. W. Gill,
Phys. Rev. A, **2010**, *81*, 052510.
22. Electronic absorption spectroscopy of Ru(II) polypyridyl DNA intercalators: a theoretical study,
D. Ambrosek, **P. F. Loos**, X. Assfeld and C. Daniel, *J. Inorg. Biochem.*, **2010**, *104*, 893.
21. Hooke's law correlation in two-electron systems,
P. F. Loos*,
Phys. Rev. A, **2010**, *81*, 032510.
20. Electronic effects and ring strain influences on the electron uptake by selenium-containing bonds,
E. Dumont, **P. F. Loos**, A. D. Laurent and X. Assfeld,
Int. J. Quantum Chem., **2010**, *110*, 513.
19. Correlation energy of two electrons in the high-density limit,
P. F. Loos* and P. M. W. Gill,
J. Chem. Phys., **2009**, *131*, 241101.
18. Two electrons on a hypersphere: a quasi-exactly solvable model,
P. F. Loos and P. M. W. Gill,
Phys. Rev. Lett., **2009**, *103*, 123008.
17. Ground state of two electrons on a sphere,
P. F. Loos and P. M. W. Gill,
Phys. Rev. A, **2009**, *79*, 062517.
16. Important effects of neighboring nucleotides on electron induced DNA single-strand breaks,
P. F. Loos*, E. Dumont, A. D. Laurent and X. Assfeld,
Chem. Phys. Lett., **2009**, *475*, 120.

15. Analyzing the selectivity and successiveness of a two-electron capture on a multiply disulfide-linked protein,
E. Dumont, A. D. Laurent, **P. F. Loos** and X. Assfeld,
J. Chem. Theor. Comput., **2009**, 5, 1700.
14. Factors governing electron capture by small disulfide loops in two-cysteines peptides,
E. Dumont, **P. F. Loos** and X. Assfeld,
J. Phys. Chem. B, **2008**, 112, 13661.
13. Huge disulfide-linkage's reducible potential variation induced by α -helix orientation,
E. Dumont, **P. F. Loos**, A. D. Laurent and X. Assfeld,
J. Chem. Theor. Comput., **2008**, 4, 1171.
12. Effect of ring strain on disulfide electron attachment,
E. Dumont, **P. F. Loos** and X. Assfeld,
Chem. Phys. Lett., **2008**, 458, 276.
11. Theoretical investigation of the geometries and UV/Vis spectra of Poly(L-glutamic acid) featuring photochromic azobenzene side chain,
P. F. Loos^{*}, J. Preat, A. Laurent, C. Michaux, D. Jacquemin, E. A. Perpete and X. Assfeld,
J. Chem. Theor. Comput., **2008**, 4, 637.
10. On the frontier bond location in the QM/MM description of the peptides and proteins,
P. F. Loos and X. Assfeld,
AIP Conf. Proc., **2007**, 963, 308.
9. Removing the extra frontier parameters in QM/MM methods: a tentative with the Local Self-Consistent Field approach,
P. F. Loos, A. Fornili, M. Sironi and X. Assfeld,
Comput. Lett. **2007**, 4, 473.
8. Core-ionized and core-excited states of macromolecules,
P. F. Loos and X. Assfeld,
Int. J. Quantum Chem., **2007**, 107, 2343.
7. A TD-DFT investigation of UV spectra of pyranoïdic dyes: a NCM vs. PCM comparison,
J. Preat, **P. F. Loos**, X. Assfeld, D. Jacquemin and E. A. Perpete,
J. Mol. Struct. (THEOCHEM), **2007**, 808, 85.
6. Self-Consistent Strictly Localized Orbitals,
P. F. Loos and X. Assfeld,
J. Chem. Theor. Comput., **2007**, 3, 1047.
5. Intramolecular interactions and cis peptidic bonds,
P. F. Loos, X. Assfeld and J.-L. Rivail,
Theor. Chem. Acc., **2007**, 118, 165.
4. DFT and TD-DFT investigation of IR and UV spectra of solvated molecules: comparison of two SCRF continuum models,
J. Preat, **P. F. Loos**, X. Assfeld, D. Jacquemin and E. A. Perpete,
Int. J. Quantum Chem., **2007**, 107, 574.

3. Electronic factors favouring the cis conformation in proline peptidic bonds,
J.-L. Rivail, A. Bouchy and **P. F. Loos**,
J. Argentine Chem. Soc., **2006**, 94, 19.
2. Frozen core orbitals as an alternative to specific frontier bond potential in hybrid Quantum Mechanics/Molecular Mechanics methods,
A. Fornili, **P. F. Loos**, X. Assfeld and M. Sironi,
Chem. Phys. Lett., **2006**, 427, 236.
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,
Y. Moreau, **P. F. Loos** and X. Assfeld,
Theor. Chem. Acc., **2004**, 112, 228.