Julien Toulouse

List of Publications by Year in descending order

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84 papers	4,640 citations	126907 33 h-index	98798 67 g-index
86 all docs	86 docs citations	86 times ranked	2028 citing authors

#	Article	IF	Citations
1	Alleviation of the Fermion-Sign Problem by Optimization of Many-Body Wave Functions. Physical Review Letters, 2007, 98, 110201.	7.8	411
2	Long-rangeâ€“short-range separation of the electron-electron interaction in density-functional theory. Physical Review A, 2004, 70, .	2.5	381
3	van der Waals forces in density functional theory: Perturbational long-range electron-interaction corrections. Physical Review A, 2005, 72, .	2.5	287
4	Adiabatic-Connection Fluctuation-Dissipation Density-Functional Theory Based on Range Separation. Physical Review Letters, 2009, 102, 096404.	7.8	240
5	Optimization of quantum Monte Carlo wave functions by energy minimization. Journal of Chemical Physics, 2007, 126, 084102.	3.0	226
6	On the universality of the long-/short-range separation in multiconfigurational density-functional theory. Journal of Chemical Physics, 2007, 126, 074111.	3.0	171
7	Full optimization of Jastrowâ€“Slater wave functions with application to the first-row atoms and homonuclear diatomic molecules. Journal of Chemical Physics, 2008, 128, 174101.	3.0	167
8	Double-hybrid density-functional theory made rigorous. Journal of Chemical Physics, 2011, 134, 064113.	3.0	165
9	Correlation Energy Expressions from the Adiabatic-Connection Fluctuationâ€“Dissipation Theorem Approach. Journal of Chemical Theory and Computation, 2011, 7, 3116-3130.	5.3	122
10	Short-range exchange and correlation energy density functionals: Beyond the local-density approximation. Journal of Chemical Physics, 2005, 122, 014110.	3.0	120
11	Range-separated density-functional theory with random phase approximation applied to noncovalent intermolecular interactions. Journal of Chemical Physics, 2010, 132, 244108.	3.0	119
12	Short-range exchange-correlation energy of a uniform electron gas with modified electron-electron interaction. International Journal of Quantum Chemistry, 2004, 100, 1047-1056.	2.0	115
13	Range-separated density-functional theory with the random-phase approximation: Detailed formalism and illustrative applications. Physical Review A, 2010, 82, .	2.5	115
14	Quantum Package 2.0: An Open-Source Determinant-Driven Suite of Programs. Journal of Chemical Theory and Computation, 2019, 15, 3591-3609.	5.3	108
15	Blind test of density-functional-based methods on intermolecular interaction energies. Journal of Chemical Physics, 2016, 145, 124105.	3.0	97
16	Communication: Rationale for a new class of double-hybrid approximations in density-functional theory. Journal of Chemical Physics, 2011, 135, 101102.	3.0	93
17	Closed-shell ring coupled cluster doubles theory with range separation applied on weak intermolecular interactions. Journal of Chemical Physics, 2011, 135, 084119.	3.0	85
18	Validation and assessment of an accurate approach to the correlation problem in density functional theory: The Krigerâ€“Chenâ€“Iafrateâ€“Savin model. Journal of Chemical Physics, 2002, 117, 10465-10473.	3.0	83

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19	A multiconfigurational hybrid density-functional theory. Journal of Chemical Physics, 2012, 137, 044104.	3.0	77
20	Excited states of methylene from quantum Monte Carlo. Journal of Chemical Physics, 2009, 131, 124103.	3.0	70
21	Approaching chemical accuracy with quantum Monte Carlo. Journal of Chemical Physics, 2012, 136, 124116.	3.0	70
22	A short-range correlation energy density functional with multi-determinantal reference. Theoretical Chemistry Accounts, 2005, 114, 305-308.	1.4	45
23	Combining density-functional theory and density-matrix-functional theory. Physical Review A, 2010, 82, .	2.5	45
24	Introduction to the Variational and Diffusion Monte Carlo Methods. Advances in Quantum Chemistry, 2016, 73, 285-314.	0.8	45
25	Quantum Monte Carlo with Jastrow-valence-bond wave functions. Journal of Chemical Physics, 2011, 134, 084108.	3.0	43
26	Kohn-Sham potentials in exact density-functional theory at noninteger electron numbers. Physical Review A, 2014, 90, .	2.5	42
27	Almost exact energies for the Gaussian-2 set with the semistochastic heat-bath configuration interaction method. Journal of Chemical Physics, 2020, 153, 124117.	3.0	41
28	Basis convergence of range-separated density-functional theory. Journal of Chemical Physics, 2015, 142, 074107.	3.0	40
29	Alternative separation of exchange and correlation energies in multi-configuration range-separated density-functional theory. Journal of Chemical Physics, 2013, 139, 134113.	3.0	37
30	Double-hybrid density-functional theory with meta-generalized-gradient approximations. Journal of Chemical Physics, 2014, 140, 084107.	3.0	35
31	Multiconfigurational short-range density-functional theory for open-shell systems. Journal of Chemical Physics, 2018, 148, 214103.	3.0	35
32	Spin-unrestricted random-phase approximation with range separation: Benchmark on atomization energies and reaction barrier heights. Journal of Chemical Physics, 2015, 142, 154123.	3.0	34
33	Range-separated multideterminant density-functional theory with a short-range correlation functional of the on-top pair density. Journal of Chemical Physics, 2019, 150, 084103.	3.0	34
34	A general range-separated double-hybrid density-functional theory. Journal of Chemical Physics, 2018, 148, 164105.	3.0	33
35	Curing basis-set convergence of wave-function theory using density-functional theory: A systematically improvable approach. Journal of Chemical Physics, 2018, 149, 194301.	3.0	33
36	Zero-variance zero-bias quantum Monte Carlo estimators of the spherically and system-averaged pair density. Journal of Chemical Physics, 2007, 126, 244112.	3.0	32

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37	Gaussian continuum basis functions for calculating high-harmonic generation spectra. International Journal of Quantum Chemistry, 2016, 116, 1120-1131.	2.0	32
38	Chemically accurate excitation energies with small basis sets. Journal of Chemical Physics, 2019, 151, 144118.	3.0	30
39	Range-separated time-dependent density-functional theory with a frequency-dependent second-order Bethe-Salpeter correlation kernel. Journal of Chemical Physics, 2016, 144, 094107.	3.0	28
40	Optimal Basis Set for Electron Dynamics in Strong Laser Fields: The case of Molecular Ion H₂⁺. Journal of Chemical Theory and Computation, 2018, 14, 5846-5858.	5.3	28
41	A new hybrid functional including a meta-GGA approach. Chemical Physics Letters, 2002, 362, 72-78.	2.6	26
42	Ab initio lifetime correction to scattering states for time-dependent electronic-structure calculations with incomplete basis sets. Journal of Chemical Physics, 2017, 147, 014106.	3.0	26
43	A Density-Based Basis-Set Correction for Wave Function Theory. Journal of Physical Chemistry Letters, 2019, 10, 2931-2937.	4.6	26
44	Self-consistent double-hybrid density-functional theory using the optimized-effective-potential method. Journal of Chemical Physics, 2016, 145, 144102.	3.0	25
45	Local density approximation for long-range or for short-range energy functionals?. Computational and Theoretical Chemistry, 2006, 762, 147-150.	1.5	24
46	Double-hybrid density-functional theory applied to molecular crystals. Journal of Chemical Physics, 2014, 141, 044105.	3.0	24
47	Density-Based Basis-Set Incompleteness Correction for GW Methods. Journal of Chemical Theory and Computation, 2020, 16, 1018-1028.	5.3	24
48	Electronic excitations from a linear-response range-separated hybrid scheme. Molecular Physics, 2013, 111, 1219-1234.	1.7	23
49	Quantum Monte Carlo with reoptimised perturbatively selected configuration-interaction wave functions. Molecular Physics, 2016, 114, 910-920.	1.7	22
50	Scaling relations, virial theorem, and energy densities for long-range and short-range density functionals. International Journal of Quantum Chemistry, 2006, 106, 2026-2034.	2.0	21
51	Range-separated double-hybrid density-functional theory applied to periodic systems. Journal of Chemical Physics, 2015, 143, 102811.	3.0	21
52	Fractional-charge and fractional-spin errors in range-separated density-functional theory. Molecular Physics, 2017, 115, 161-173.	1.7	21
53	Assessment of range-separated time-dependent density-functional theory for calculating C6 dispersion coefficients. Journal of Chemical Physics, 2013, 138, 194106.	3.0	20
54	Range-separated double-hybrid density-functional theory with coupled-cluster and random-phase approximations. Journal of Chemical Physics, 2019, 151, 074102.	3.0	20

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55	A formally exact one-frequency-only Bethe-Salpeter-like equation. Similarities and differences between GW +BSE and self-consistent RPA. Journal of Chemical Physics, 2019, 150, 084112.	3.0	20
56	Simple model of the static exchange-correlation kernel of a uniform electron gas with long-range electron-electron interaction. Physical Review B, 2005, 72, .	3.2	18
57	Excitation energies along a range-separated adiabatic connection. Journal of Chemical Physics, 2014, 141, 044123.	3.0	17
58	A basis-set error correction based on density-functional theory for strongly correlated molecular systems. Journal of Chemical Physics, 2020, 152, 174104.	3.0	16
59	About the collapse of the 3.3â€‚Î¼m CH stretching band with ionization in polycyclic aromatic hydrocarbons: Configuration interaction and quantum Monte Carlo studies of the CH fragment. Journal of Chemical Physics, 2010, 133, 054301.	3.0	15
60	Basis set construction for molecular electronic structure theory: Natural orbital and Gaussâ€“Slater basis for smooth pseudopotentials. Journal of Chemical Physics, 2011, 134, 064104.	3.0	15
61	Self-Consistent Range-Separated Density-Functional Theory with Second-Order Perturbative Correction via the Optimized-Effective-Potential Method. Journal of Chemical Theory and Computation, 2020, 16, 211-223.	5.3	15
62	Calculating excitation energies by extrapolation along adiabatic connections. Physical Review A, 2015, 91, .	2.5	14
63	Four-component relativistic range-separated density-functional theory: Short-range exchange local-density approximation. Journal of Chemical Physics, 2018, 149, 174110.	3.0	14
64	Asymptotic behavior of the Hartree-exchange and correlation potentials in ensemble density functional theory. Physical Chemistry Chemical Physics, 2019, 21, 19805-19815.	2.8	14
65	Linear-response range-separated density-functional theory for atomic photoexcitation and photoionization spectra. Journal of Chemical Physics, 2019, 150, 234104.	3.0	13
66	Exchangeâ€“correlation potentials and local energies per particle along nonlinear adiabatic connections. Molecular Physics, 2005, 103, 2725-2734.	1.7	12
67	Excited states from range-separated density-functional perturbation theory. Molecular Physics, 2015, 113, 1740-1749.	1.7	12
68	Quantum Monte Carlo study of the cooperative binding of NO2 to fragment models of carbon nanotubes. Chemical Physics Letters, 2008, 466, 170-175.	2.6	9
69	Self-consistent density-based basis-set correction: How much do we lower total energies and improve dipole moments?. Journal of Chemical Physics, 2021, 155, 044109.	3.0	9
70	Accurate energies of transition metal atoms, ions, and monoxides using selected configuration interaction and density-based basis-set corrections. Journal of Chemical Physics, 2021, 155, 204104.	3.0	9
71	Compact and flexible basis functions for quantum Monte Carlo calculations. Journal of Chemical Physics, 2010, 132, 094109.	3.0	8
72	Casimirâ€“Polder Size Consistency: A Constraint Violated by Some Dispersion Theories. Journal of Chemical Theory and Computation, 2017, 13, 5829-5833.	5.3	8

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73	Relativistic short-range exchange energy functionals beyond the local-density approximation. Journal of Chemical Physics, 2020, 152, 214106.	3.0	8
74	Time-Dependent Linear-Response Variational Monte Carlo. Advances in Quantum Chemistry, 2018, 76, 255-270.	0.8	6
75	Basis-set correction based on density-functional theory: Rigorous framework for a one-dimensional model. Journal of Chemical Physics, 2022, 156, 044113.	3.0	6
76	Excitation energies from GÃ¶rlingâ€“Levy perturbation theory along the range-separated adiabatic connection. Molecular Physics, 2018, 116, 1443-1451.	1.7	5
77	Relativistic density-functional theory based on effective quantum electrodynamics. , 2021, 1, .		5
78	Quantum Monte Carlo Calculations of Electronic Excitation Energies: The Case of the Singlet nâ†'Ï€â^— (CO) Transition in Acrolein. Progress in Theoretical Chemistry and Physics, 2012, , 343-351.	0.2	5
79	Basis-set correction for coupled-cluster estimation of dipole moments. Journal of Chemical Physics, 2022, 156, 174101.	3.0	4
80	Photoionization and core resonances from range-separated density-functional theory: General formalism and example of the beryllium atom. Journal of Chemical Physics, 2022, 156, .	3.0	4
81	Shortâ€range correlation energy of the relativistic homogeneous electron gas. International Journal of Quantum Chemistry, 2021, 121, e26685.	2.0	3
82	Quantum Monte Carlo Facing the Hartree-Fock Symmetry Dilemma: The Case of Hydrogen Rings. ACS Symposium Series, 2012, , 53-63.	0.5	2
83	Range-separated density-functional theory applied to the beryllium dimer and trimer. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	2
84	Foreword for special issue of Molecular Physics in honour of Andreas Savin. Molecular Physics, 2016, 114, 909-909.	1.7	0