Emmanuel Fromager

List of Publications by Year
in descending order

48 papers	1,218 citations	331670 21 h-index	377865 34 g-index
49 all docs	49 docs citations	49 times ranked	665 citing authors

#	Article	IF	Citations
1	On the universality of the long-/short-range separation in multiconfigurational density-functional theory. Journal of Chemical Physics, 2007, 126, 074111.	3.0	171
2	Multi-configuration time-dependent density-functional theory based on range separation. Journal of Chemical Physics, 2013, 138, 084101.	3.0	88
3	Merging multireference perturbation and density-functional theories by means of range separation: Potential curves for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Be</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Mg</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></m	2.5	60
4	Self-consistent many-body perturbation theory in range-separated density-functional theory: A one-electron reduced-density-matrix-based formulation. Physical Review A, 2008, 78, .	2.5	56
5	On the universality of the long-/short-range separation in multiconfigurational density-functional theory. II. Investigating f actinide species. Journal of Chemical Physics, 2009, 131, 054107.	3.0	49
6	Generalised adiabatic connection in ensemble density-functional theory for excited states: example of the H₂ molecule. Molecular Physics, 2014, 112, 1684-1701.	1.7	49
7	On the exact formulation of multi-configuration density-functional theory: electron density versus orbitals occupation. Molecular Physics, 2015, 113, 419-434.	1.7	47
8	Rigorous formulation of two-parameter double-hybrid density-functionals. Journal of Chemical Physics, 2011, 135, 244106.	3.0	43
9	Analysis of double-hybrid density functionals along the adiabatic connection. Molecular Physics, 2013, 111, 1275-1294.	1.7	42
10	Assessment of charge-transfer excitations with time-dependent, range-separated density functional theory based on long-range MP2 and multiconfigurational self-consistent field wave functions. Journal of Chemical Physics, 2013, 139, 184308.	3.0	39
11	Electron Transfer in Uranyl(VI)â^'Uranyl(V) Complexes in Solution. Journal of the American Chemical Society, 2004, 126, 9801-9808.	13.7	37
12	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
13	Exact ensemble density functional theory for excited states in a model system: Investigating the weight dependence of the correlation energy. Physical Review B, 2017, 95, .	3.2	36
14	Unified formulation of fundamental and optical gap problems in density-functional theory for ensembles. Physical Review A, 2018, 98, .	2.5	33
15	Local density approximation in site-occupation embedding theory. Molecular Physics, 2017, 115, 48-62.	1.7	31
16	Ground and excited energy levels can be extracted exactly from a single ensemble density-functional theory calculation. Journal of Chemical Physics, 2019, 150, 094106.	3.0	31
17	Linear interpolation method in ensemble Kohn-Sham and range-separated density-functional approximations for excited states. Physical Review A, 2015, 92, .	2.5	27
18	Double hybrid densityâ€functional theory using the coulombâ€attenuating method. International Journal of Quantum Chemistry, 2014, 114, 1199-1211.	2.0	26

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19	Individual Correlations in Ensemble Density Functional Theory: State- and Density-Driven Decompositions without Additional Kohn-Sham Systems. Physical Review Letters, 2020, 124, 243001.	7.8	23
20	A weight-dependent local correlation density-functional approximation for ensembles. Journal of Chemical Physics, 2020, 152, 214101.	3.0	22
21	Site-occupation embedding theory using Bethe ansatz local density approximations. Physical Review B, 2018, 97, .	3.2	21
22	Nâ€centered ensemble densityâ€functional theory for open systems. International Journal of Quantum Chemistry, 2020, 120, e26190.	2.0	20
23	Weight dependence of local exchangeâ€“correlation functionals in ensemble density-functional theory: double excitations in two-electron systems. Faraday Discussions, 2020, 224, 402-423.	3.2	19
24	Alternative separation of exchange and correlation energies in range-separated density-functional perturbation theory. Physical Review A, 2013, 88, .	2.5	16
25	Ghost-interaction correction in ensemble density-functional theory for excited states with and without range separation. Physical Review A, 2016, 94, .	2.5	16
26	Combining linear interpolation with extrapolation methods in range-separated ensemble density functional theory. Molecular Physics, 2016, 114, 968-981.	1.7	15
27	Exploring weight-dependent density-functional approximations for ensembles in the Hubbard dimer. European Physical Journal B, 2018, 91, 1.	1.5	15
28	Spinâ^'Orbit Effects in Electron Transfer in Neptunyl(VI)â^'Neptunyl(V) Complexes in Solution. Journal of Physical Chemistry A, 2005, 109, 4957-4960.	2.5	14
29	Foreword for the special issue of Molecular Physics in honour of Hans JÃ¸rgen Aagaard Jensen. Molecular Physics, 2017, 115, 1-4.	1.7	13
30	Analysis of self-consistency effects in range-separated density-functional theory with MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2011, 135, 034116.	3.0	12
31	Metallophilic interactions in A-frame molecules [S(MPH3)2] (M=Cu, Ag, Au) from range-separated density-functional perturbation theory. Chemical Physics Letters, 2012, 554, 37-42.	2.6	12
32	Ensemble Density Functional Theory of Neutral and Charged Excitations. Topics in Current Chemistry, 2022, 380, 4.	5.8	12
33	Electron Transfer in Neptunyl(VI)â^'Neptunyl(V) Complexes in Solution. Journal of Physical Chemistry A, 2005, 109, 4950-4956.	2.5	11
34	Combining extrapolation with ghost interaction correction in range-separated ensemble density functional theory for excited states. Journal of Chemical Physics, 2017, 147, 204105.	3.0	11
35	An analysis of core effects on shape-consistent pseudopotentials. Journal of Chemical Physics, 2004, 121, 8687-8698.	3.0	10
36	Electron transport through a spin crossover junction. Perspectives from a wavefunction-based approach. Journal of Chemical Physics, 2017, 146, 064112.	3.0	9

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37	Householder-transformed density matrix functional embedding theory. Physical Review B, 2021, 104, .	3.2	9
38	Multiple impurities and combined local density approximations in site-occupation embedding theory. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	8
39	Atomic spin-orbit pseudopotential definition and its relation to the different relativistic approximations. Journal of Chemical Physics, 2005, 123, 034106.	3.0	6
40	Local Potential Functional Embedding Theory: A Self-Consistent Flavor of Density Functional Theory for Lattices without Density Functionals. Computation, 2022, 10, 45.	2.0	6
41	On the accuracy of one-component pseudopotential spin-orbit calculations. Journal of Chemical Physics, 2005, 123, 164105.	3.0	4
42	Site-occupation Green's function embedding theory: A density functional approach to dynamical impurity solvers. Physical Review B, 2019, 100, .	3.2	4
43	Exact exchange-correlation potentials for calculating the fundamental gap with a fixed number of electrons. Physical Review A, 2021, 103, .	2.5	3
44	Strong correlation in density functional theory: general discussion. Faraday Discussions, 2020, 224, 373-381.	3.2	2
45	New approaches to study excited states in density functional theory: general discussion. Faraday Discussions, 2020, 224, 483-508.	3.2	2
46	New density-functional approximations and beyond: general discussion. Faraday Discussions, 2020, 224, 166-200.	3.2	1
47	Electron Transfer in Uranyl(VI)-Uranyl(V) Complexes in Solution.. ChemInform, 2004, 35, no.	0.0	0
48	Extraction of shape-consistent spin-orbit pseudo-potential from an effective spin-orbit parameter and application to the tellurium atom. International Journal of Quantum Chemistry, 2006, 106, 764-771.	2.0	0