

Oleg Gritsenko

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38

papers

3,399

citations

20

h-index

43

g-index

43

ext. papers

3,569

ext. citations

3.5

avg, IF

5.14

L-index

#	Paper	IF	Citations
38	Molecular calculations of excitation energies and (hyper)polarizabilities with a statistical average of orbital model exchange-correlation potentials. <i>Journal of Chemical Physics</i> , 2000 , 112, 1344-1352	3.9	646
37	A Quantum Chemical View of Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 1997 , 101, 5383-5403	5.11	511
36	Interpretation of the Kohn-Sham orbital energies as approximate vertical ionization potentials. <i>Journal of Chemical Physics</i> , 2002 , 116, 1760-1772	3.9	433
35	Electric Field Dependence of the Exchange-Correlation Potential in Molecular Chains. <i>Physical Review Letters</i> , 1999 , 83, 694-697	7.4	326
34	Density-functional-theory response-property calculations with accurate exchange-correlation potentials. <i>Physical Review A</i> , 1998 , 57, 2556-2571	2.6	231
33	Improved density functional theory results for frequency-dependent polarizabilities, by the use of an exchange-correlation potential with correct asymptotic behavior. <i>Journal of Chemical Physics</i> , 1996 , 105, 3142-3151	3.9	184
32	An improved density matrix functional by physically motivated repulsive corrections. <i>Journal of Chemical Physics</i> , 2005 , 122, 204102	3.9	158
31	Physical Meaning of Virtual Kohn-Sham Orbitals and Orbital Energies: An Ideal Basis for the Description of Molecular Excitations. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 4432-41	6.4	155
30	Excitation energies of dissociating H ₂ : A problematic case for the adiabatic approximation of time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2000 , 113, 8478-8489	3.9	88
29	A density matrix functional with occupation number driven treatment of dynamical and nondynamical correlation. <i>Journal of Chemical Physics</i> , 2008 , 129, 164105	3.9	87
28	Time-dependent density-matrix-functional theory. <i>Physical Review A</i> , 2007 , 75,	2.6	76
27	The spin-unrestricted molecular Kohn-Sham solution and the analogue of Koopmans's theorem for open-shell molecules. <i>Journal of Chemical Physics</i> , 2004 , 120, 8364-72	3.9	75
26	Kohn-Sham potentials and exchange and correlation energy densities from one- and two-electron density matrices for Li ₂ , N ₂ , and F ₂ . <i>Physical Review A</i> , 1998 , 57, 1729-1742	2.6	53
25	Excitation energies with time-dependent density matrix functional theory: Singlet two-electron systems. <i>Journal of Chemical Physics</i> , 2009 , 130, 114104	3.9	50
24	Exchange-correlation energy and potential as approximate functionals of occupied and virtual Kohn-Sham orbitals: Application to dissociating H ₂ . <i>Journal of Chemical Physics</i> , 2003 , 118, 7183	3.9	47
23	On the errors of local density (LDA) and generalized gradient (GGA) approximations to the Kohn-Sham potential and orbital energies. <i>Journal of Chemical Physics</i> , 2016 , 144, 204114	3.9	39
22	Response calculations with an independent particle system with an exact one-particle density matrix. <i>Physical Review Letters</i> , 2010 , 105, 013002	7.4	38

21	Adiabatic approximation of time-dependent density matrix functional response theory. <i>Journal of Chemical Physics</i> , 2007 , 127, 214101	3.9	37
20	The density matrix functional approach to electron correlation: dynamic and nondynamic correlation along the full dissociation coordinate. <i>Journal of Chemical Physics</i> , 2014 , 140, 214105	3.9	24
19	The analog of Koopmans's theorem for virtual Kohn-Sham orbital energies. <i>Canadian Journal of Chemistry</i> , 2009 , 87, 1383-1391	0.9	24
18	Efficient evaluation of electron correlation along the bond-dissociation coordinate in the ground and excited ionic states with dynamic correlation suppression and enhancement functions of the on-top pair density. <i>Physical Review A</i> , 2018 , 98,	2.6	16
17	A non-JKL density matrix functional for intergeminal correlation between closed-shell geminals from analysis of natural orbital configuration interaction expansions. <i>Journal of Chemical Physics</i> , 2018 , 148, 104102	3.9	14
16	Excitation energies with linear response density matrix functional theory along the dissociation coordinate of an electron-pair bond in N-electron systems. <i>Journal of Chemical Physics</i> , 2014 , 140, 024101	3.9	14
15	Natural excitation orbitals from linear response theories: Time-dependent density functional theory, time-dependent Hartree-Fock, and time-dependent natural orbital functional theory. <i>Journal of Chemical Physics</i> , 2017 , 146, 044119	3.9	9
14	Comment on "Kohn-Sham exchange-correlation potentials from second-order reduced density matrices" [J. Chem. Phys. 143, 244116 (2015)]. <i>Journal of Chemical Physics</i> , 2016 , 145, 037101	3.9	9
13	Complete active space and corrected density functional theories helping each other to describe vertical electronic excitations in prototype multiple-bonded molecules. <i>Journal of Chemical Physics</i> , 2019 , 151, 024111	3.9	7
12	Approximating one-matrix functionals without generalized Pauli constraints. <i>Physical Review A</i> , 2019 , 100,	2.6	7
11	On the formulation of a density matrix functional for Van der Waals interaction of like- and opposite-spin electrons in the helium dimer. <i>Journal of Chemical Physics</i> , 2012 , 137, 204117	3.9	7
10	Electron correlation energy with a combined complete active space and corrected density-functional approach in a small basis versus the reference complete basis set limit: A close agreement. <i>Chemical Physics Letters</i> , 2019 , 716, 227-230	2.5	7
9	Reproducing benchmark potential energy curves of molecular bond dissociation with small complete active space aided with density and density-matrix functional corrections. <i>Journal of Chemical Physics</i> , 2019 , 151, 164122	3.9	6
8	Response calculations based on an independent particle system with the exact one-particle density matrix: polarizabilities. <i>Journal of Chemical Physics</i> , 2014 , 140, 18A517	3.9	6
7	Local Enhancement of Dynamic Correlation in Excited States: Fresh Perspective on Ionicity and Development of Correlation Density Functional Approximation Based on the On-Top Pair Density. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 5883-5889	6.4	5
6	Time-dependent Dyson orbital theory. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 20945-54	3.6	3
5	Correlation-coupling entropy as a measure of strong electron correlation and fragment-conditional density spin polarization as a measure of electron entanglement. <i>Physical Review A</i> , 2019 , 100,	2.6	2
4	Molecular multibond dissociation with small complete active space augmented by correlation density functionals. <i>Journal of Chemical Physics</i> , 2020 , 152, 204118	3.9	2

3	Combining density-based dynamical correlation with a reduced-density-matrix strong-correlation description. <i>Physical Review A</i> , 2020 , 102,	2.6	2
2	Bond-breaking excitations with diverging coupling matrix of response density functional theory from highest-level functionals. <i>European Physical Journal B</i> , 2018 , 91, 1	1.2	0
1	Embracing local suppression and enhancement of dynamic correlation effects in a CASDFT method for efficient description of excited states. <i>Faraday Discussions</i> , 2020 , 224, 333-347	3.6	0