Oleg Gritsenko

List of Publications by Year in Descending Order

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 multibond dissociation with small complete active space augmented by correlation density functionals. *Journal of Chemical Physics*, **2020**, 152, 204118	3.9	2
37	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. *Journal of Physical Chemistry Letters*, **2020**, 11, 5883-5889	6.4	5
36	Embracing local suppression and enhancement of dynamic correlation effects in a CASDFT method for efficient description of excited states. *Faraday Discussions*, **2020**, 224, 333-347	3.6	0
35	Combining density-based dynamical correlation with a reduced-density-matrix strong-correlation description. *Physical Review A*, **2020**, 102,	2.6	2
34	Correlation-coupling entropy as a measure of strong electron correlation and fragment-conditional density spin polarization as a measure of electron entanglement. *Physical Review A*, **2019**, 100,	2.6	2
33	Complete active space and corrected density functional theories helping each other to describe vertical electronic ¹,³Σ⁺u excitations in prototype multiple-bonded molecules. *Journal of Chemical Physics*, **2019**, 151, 024111	3.9	7
32	Approximating one-matrix functionals without generalized Pauli constraints. *Physical Review A*, **2019**, 100,	2.6	7
31	Reproducing benchmark potential energy curves of molecular bond dissociation with small complete active space aided with density and density-matrix functional corrections. *Journal of Chemical Physics*, **2019**, 151, 164122	3.9	6
30	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. *Chemical Physics Letters*, **2019**, 716, 227-230	2.5	7
29	A non-JKL density matrix functional for intergeminal correlation between closed-shell geminals from analysis of natural orbital configuration interaction expansions. *Journal of Chemical Physics*, **2018**, 148, 104102	3.9	14
28	Bond-breaking excitations with diverging coupling matrix of response density functional theory from highest-level functionals. *European Physical Journal B*, **2018**, 91, 1	1.2	0
27	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. *Physical Review A*, **2018**, 98,	2.6	16
26	Natural excitation orbitals from linear response theories: Time-dependent density functional theory, time-dependent Hartree-Fock, and time-dependent natural orbital functional theory. *Journal of Chemical Physics*, **2017**, 146, 044119	3.9	9
25	Time-dependent Dyson orbital theory. *Physical Chemistry Chemical Physics*, **2016**, 18, 20945-54	3.6	3
24	Comment on "Kohn-Sham exchange-correlation potentials from second-order reduced density matrices" [J. Chem. Phys. 143, 244116 (2015)]. *Journal of Chemical Physics*, **2016**, 145, 037101	3.9	9
23	On the errors of local density (LDA) and generalized gradient (GGA) approximations to the Kohn-Sham potential and orbital energies. *Journal of Chemical Physics*, **2016**, 144, 204114	3.9	39
22	Excitation energies with linear response density matrix functional theory along the dissociation coordinate of an electron-pair bond in N-electron systems. *Journal of Chemical Physics*, **2014**, 140, 024101	3.9	14

21	Physical Meaning of Virtual Kohn-Sham Orbitals and Orbital Energies: An Ideal Basis for the Description of Molecular Excitations. *Journal of Chemical Theory and Computation*, **2014**, 10, 4432-41	6.4	155
20	The density matrix functional approach to electron correlation: dynamic and nondynamic correlation along the full dissociation coordinate. *Journal of Chemical Physics*, **2014**, 140, 214105	3.9	24
19	Response calculations based on an independent particle system with the exact one-particle density matrix: polarizabilities. *Journal of Chemical Physics*, **2014**, 140, 18A517	3.9	6
18	On the formulation of a density matrix functional for Van der Waals interaction of like- and opposite-spin electrons in the helium dimer. *Journal of Chemical Physics*, **2012**, 137, 204117	3.9	7
17	Response calculations with an independent particle system with an exact one-particle density matrix. *Physical Review Letters*, **2010**, 105, 013002	7.4	38
16	Excitation energies with time-dependent density matrix functional theory: Singlet two-electron systems. *Journal of Chemical Physics*, **2009**, 130, 114104	3.9	50
15	The analog of Koopmans□theorem for virtual Kohn□Sham orbital energies. *Canadian Journal of Chemistry*, **2009**, 87, 1383-1391	0.9	24
14	A density matrix functional with occupation number driven treatment of dynamical and nondynamical correlation. *Journal of Chemical Physics*, **2008**, 129, 164105	3.9	87
13	Adiabatic approximation of time-dependent density matrix functional response theory. *Journal of Chemical Physics*, **2007**, 127, 214101	3.9	37
12	Time-dependent density-matrix-functional theory. *Physical Review A*, **2007**, 75,	2.6	76
11	An improved density matrix functional by physically motivated repulsive corrections. *Journal of Chemical Physics*, **2005**, 122, 204102	3.9	158
10	The spin-unrestricted molecular Kohn-Sham solution and the analogue of Koopmans's theorem for open-shell molecules. *Journal of Chemical Physics*, **2004**, 120, 8364-72	3.9	75
9	Exchange-correlation energy and potential as approximate functionals of occupied and virtual Kohn□Sham orbitals: Application to dissociating H[sub 2]. *Journal of Chemical Physics*, **2003**, 118, 7183	3.9	47
8	Interpretation of the Kohn□Sham orbital energies as approximate vertical ionization potentials. *Journal of Chemical Physics*, **2002**, 116, 1760-1772	3.9	433
7	Molecular calculations of excitation energies and (hyper)polarizabilities with a statistical average of orbital model exchange-correlation potentials. *Journal of Chemical Physics*, **2000**, 112, 1344-1352	3.9	646
6	Excitation energies of dissociating H2: A problematic case for the adiabatic approximation of time-dependent density functional theory. *Journal of Chemical Physics*, **2000**, 113, 8478-8489	3.9	88
5	Electric Field Dependence of the Exchange-Correlation Potential in Molecular Chains. *Physical Review Letters*, **1999**, 83, 694-697	7.4	326
4	Density-functional-theory response-property calculations with accurate exchange-correlation potentials. *Physical Review A*, **1998**, 57, 2556-2571	2.6	231

3	Kohn-Sham potentials and exchange and correlation energy densities from one- and two-electron density matrices for Li2, N2, and F2. *Physical Review A*, **1998**, 57, 1729-1742	2.6	53
2	A Quantum Chemical View of Density Functional Theory. *Journal of Physical Chemistry A*, **1997**, 101, 5383-5403	2.5	511
1	Improved density functional theory results for frequency-dependent polarizabilities, by the use of an exchange-correlation potential with correct asymptotic behavior. *Journal of Chemical Physics*, **1996**, 105, 3142-3151	3.9	184