

Scaling down the Perdew-Zunger self-interaction corre

Journal of Chemical Physics

124, 094108

DOI: 10.1063/1.2176608

Citation Report

#	ARTICLE	IF	CITATIONS
1	Assessment of a long-range corrected hybrid functional. Journal of Chemical Physics, 2006, 125, 234109.	1.2	1,526
2	A simple method to selectively scale down the self-interaction correction. Journal of Chemical Physics, 2006, 124, 191101.	1.2	37
3	Density functionals that are one- and two- are not always many-electron self-interaction-free, as shown for H ₂ ⁺ , He ₂ ⁺ , LiH ⁺ , and Ne ₂ ⁺ . Journal of Chemical Physics, 2007, 126, 104102.	1.2	274
4	Atomic-orbital-based approximate self-interaction correction scheme for molecules and solids. Physical Review B, 2007, 75, .	1.1	150
5	Efficient tight-binding approach for the study of strongly correlated systems. Physical Review B, 2007, 76, .	1.1	20
6	One-parameter optimization of a nonempirical meta-generalized-gradient-approximation for the exchange-correlation energy. Physical Review A, 2007, 76, .	1.0	37
7	Diminished gradient dependence of density functionals: Constraint satisfaction and self-interaction correction. Journal of Chemical Physics, 2007, 126, 244107.	1.2	26
8	An Efficient LDA+U Based Tight Binding Approach. Journal of Physical Chemistry A, 2007, 111, 5665-5670.	1.1	15
9	Comparison of the electronic structures of four crystalline phases of $\text{FeP}_4\text{O}_{12}$. Physical Review B, 2007, 76, .	1.1	13
10	From Insulator to Electride: A Theoretical Model of Nanoporous Oxide $12\text{CaO} \cdot 7\text{Al}_2\text{O}_3$. Journal of the American Chemical Society, 2007, 129, 942-951.	6.6	115
11	Tests of functionals for systems with fractional electron number. Journal of Chemical Physics, 2007, 126, 154109.	1.2	559
12	Ab initio analysis of the Cope rearrangement of germacrane sesquiterpenoids. Journal of Molecular Modeling, 2008, 14, 335-342.	0.8	30
13	Orbital-dependent density functionals: Theory and applications. Reviews of Modern Physics, 2008, 80, 3-60.	16.4	1,069
14	Polarizability of molecular chains: A self-interaction correction approach. Physical Review B, 2008, 77, .	1.1	56
15	Simple charge-transfer model to explain the electrical response of hydrogen chains. Physical Review A, 2008, 78, .	1.0	20
16	Self-interaction correction and the optimized effective potential. Journal of Chemical Physics, 2008, 129, 014110.	1.2	72
17	Local-density approximation for orbital densities applied to the self-interaction correction. Journal of Chemical Physics, 2008, 128, 044105.	1.2	1
18	Hartree-Fock orbitals significantly improve the reaction barrier heights predicted by semilocal density functionals. Journal of Chemical Physics, 2008, 128, 244112.	1.2	89

#	ARTICLE	IF	CITATIONS
19	Electrical Response of Molecular Systems: The Power of Self-Interaction Corrected Kohn-Sham Theory. <i>Physical Review Letters</i> , 2008, 100, 133004.	2.9	70
20	Self-interaction correction with Wannier functions. <i>Physical Review B</i> , 2008, 77, .	1.1	33
21	Understanding and correcting the self-interaction error in the electrical response of hydrogen chains. <i>Physical Review A</i> , 2008, 77, .	1.0	52
22	Modified regional self-interaction corrected time-dependent density functional theory for core excited-state calculations. <i>Journal of Computational Chemistry</i> , 2009, 30, 2583-2593.	1.5	5
23	First-principles supercell calculations for simulating a shallow donor state in Si. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2009, 373, 3989-3993.	0.9	19
24	The exchange energy of a uniform electron gas experiencing a new, flexible range separation. <i>Chemical Physics Letters</i> , 2009, 478, 283-286.	1.2	9
25	Electronic Hyperpolarizabilities for Donor-Acceptor Molecules with Long Conjugated Bridges: Calculations versus Experiment. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10994-11001.	1.1	129
26	Coulomb-only second-order perturbation theory in long-range-corrected hybrid density functionals. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 9677.	1.3	29
27	Screened hybrid density functionals for solid-state chemistry and physics. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 443-454.	1.3	384
28	Many-electron self-interaction and spin polarization errors in local hybrid density functionals. <i>Journal of Chemical Physics</i> , 2010, 133, 134116.	1.2	83
29	Koopmans' condition for density-functional theory. <i>Physical Review B</i> , 2010, 82, .	1.1	206
30	Benchmark results for empirical post-GGA functionals: Difficult exchange problems and independent tests. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 19325.	1.3	83
31	Accurate singlet and triplet excitation energies using the Localized Hartree-Fock Kohn-Sham potential. <i>Chemical Physics</i> , 2011, 391, 19-26.	0.9	13
32	Effects of the self-interaction error in Kohn-Sham calculations: A DFT+U case study on penta-aqua uranyl(VI). <i>Computational and Theoretical Chemistry</i> , 2011, 963, 337-343.	1.1	12
33	Importance of complex orbitals in calculating the self-interaction-corrected ground state of atoms. <i>Physical Review A</i> , 2011, 84, .	1.0	75
34	Variational pseudo-self-interaction-corrected density functional approach to the description of correlated solids and molecules. <i>Physical Review B</i> , 2011, 84, .	1.1	83
35	Using complex degrees of freedom in the Kohn-Sham self-interaction correction. <i>Physical Review A</i> , 2012, 85, .	1.0	50
36	The effect of the Perdew-Zunger self-interaction correction to density functionals on the energetics of small molecules. <i>Journal of Chemical Physics</i> , 2012, 137, 124102.	1.2	89

#	ARTICLE	IF	CITATIONS
37	Self-interaction correction in a real-time Kohn-Sham scheme: Access to difficult excitations in time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2012, 137, 064117.	1.2	42
38	Constrained Density Functional Theory. <i>Chemical Reviews</i> , 2012, 112, 321-370.	23.0	454
39	Switchable Nonlinear Optical Properties of $\hat{\nu}^5$ -Monocyclopentadienylmetal Complexes: A DFT Approach. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 1970-1983.	2.5	20
40	Challenges for Density Functional Theory. <i>Chemical Reviews</i> , 2012, 112, 289-320.	23.0	1,869
41	Theoretical Toolkits for Inorganic and Bioinorganic Complexes: Their Applications and Insights. , 2013, , 1-57.		1
42	Supramolecular step in design of nonlinear optical materials: Effect of π - π stacking aggregation on hyperpolarizability. <i>Journal of Chemical Physics</i> , 2013, 139, 094310.	1.2	77
43	Assessment of Tuning Methods for Enforcing Approximate Energy Linearity in Range-Separated Hybrid Functionals. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4414-4420.	2.3	31
44	Capturing static and dynamic correlations by a combination of projected Hartree-Fock and density functional theories. <i>Journal of Chemical Physics</i> , 2013, 138, 134102.	1.2	31
45	A self-interaction-free local hybrid functional: Accurate binding energies vis-à-vis accurate ionization potentials from Kohn-Sham eigenvalues. <i>Journal of Chemical Physics</i> , 2014, 140, 18A510.	1.2	66
46	Density Functional Theory Beyond the Generalized Gradient Approximation for Surface Chemistry. <i>Topics in Current Chemistry</i> , 2014, , 25-51.	4.0	9
47	Variational, Self-Consistent Implementation of the Perdew-Zunger Self-Interaction Correction with Complex Optimal Orbitals. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5324-5337.	2.3	69
48	One-electron self-interaction and the asymptotics of the Kohn-Sham potential: an impaired relation. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14357-14367.	1.3	56
49	Comparative studies of density-functional approximations for light atoms in strong magnetic fields. <i>Physical Review A</i> , 2014, 90, .	1.0	17
50	Effect of ensemble generalization on the highest-occupied Kohn-Sham eigenvalue. <i>Journal of Chemical Physics</i> , 2015, 143, 104105.	1.2	16
51	Koopmans-Compliant Self-Interaction Corrections. <i>Advances in Atomic, Molecular and Optical Physics</i> , 2015, , 105-127.	2.3	5
52	Orbital relaxation effects on Kohn-Sham frontier orbital energies in density functional theory. <i>Journal of Chemical Physics</i> , 2015, 142, 154113.	1.2	18
53	Local Scaling Correction for Reducing Delocalization Error in Density Functional Approximations. <i>Physical Review Letters</i> , 2015, 114, 053001.	2.9	69
54	First-principles approaches for strongly correlated materials: A theoretical chemistry perspective. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 722-730.	1.0	31

#	ARTICLE	IF	CITATIONS
55	Paradox of Self-Interaction Correction. <i>Advances in Atomic, Molecular and Optical Physics</i> , 2015, , 1-14.	2.3	29
56	Thermodynamic Properties of Gaseous Ruthenium Species. <i>Journal of Physical Chemistry A</i> , 2015, 119, 4961-4971.	1.1	17
57	Synergy between pair coupled cluster doubles and pair density functional theory. <i>Journal of Chemical Physics</i> , 2015, 142, 044109.	1.2	36
58	Local hybrid functionals with orbital-free mixing functions and balanced elimination of self-interaction error. <i>Journal of Chemical Physics</i> , 2015, 142, 074112.	1.2	31
59	Complex Orbitals, Multiple Local Minima, and Symmetry Breaking in Perdewâ€Zunger Self-Interaction Corrected Density Functional Theory Calculations. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3195-3207.	2.3	54
60	Effect of Complex-Valued Optimal Orbitals on Atomization Energies with the Perdewâ€Zunger Self-Interaction Correction to Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4296-4302.	2.3	29
61	Many-electron expansion: A density functional hierarchy for strongly correlated systems. <i>Physical Review B</i> , 2016, 93, .	1.1	13
62	First-Principles Photoemission Spectroscopy of DNA and RNA Nucleobases from Koopmans-Compliant Functionals. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3948-3958.	2.3	12
63	Self-interaction error in DFT-based modelling of ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 2175-2182.	1.3	20
64	Reducing density-driven error without exact exchange. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 4793-4801.	1.3	19
65	Accurate alkynyl radical structures from density functional calculations without Hartree-Fock exchange. <i>Journal of Chemical Physics</i> , 2017, 146, 054109.	1.2	5
66	Density functional theory for modelling large molecular adsorbateâ€surface interactions: a mini-review and worked example. <i>Molecular Simulation</i> , 2017, 43, 327-345.	0.9	39
67	Self-consistent self-interaction corrected density functional theory calculations for atoms using Fermi-LÃwdin orbitals: Optimized Fermi-orbital descriptors for Liâ€Kr. <i>Journal of Chemical Physics</i> , 2017, 147, 164107.	1.2	39
68	Symmetry Breaking within Fermiâ€LÃwdin Orbital Self-Interaction Corrected Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5823-5828.	2.3	6
69	Localized orbital scaling correction for systematic elimination of delocalization error in density functional approximations. <i>National Science Review</i> , 2018, 5, 203-215.	4.6	110
70	Fermiâ€LÃwdin orbital selfâ€interaction corrected density functional theory: Ionization potentials and enthalpies of formation. <i>Journal of Computational Chemistry</i> , 2018, 39, 2463-2471.	1.5	35
71	Koopmans-Compliant Spectral Functionals for Extended Systems. <i>Physical Review X</i> , 2018, 8, .	2.8	34
72	Local hybrid functionals: Theory, implementation, and performance of an emerging new tool in quantum chemistry and beyond. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2019, 9, e1378.	6.2	95

#	ARTICLE	IF	CITATIONS
73	Perdew-Zunger self-interaction correction: How wrong for uniform densities and large- Z atoms?. Journal of Chemical Physics, 2019, 150, 174106.	1.2	35
74	The effect of self-interaction error on electrostatic dipoles calculated using density functional theory. Journal of Chemical Physics, 2019, 151, 174106.	1.2	29
75	Reducing the Many-Electron Self-Interaction Error in the Second-Order Screened Exchange Method. Journal of Chemical Theory and Computation, 2019, 15, 6607-6616.	2.3	8
76	Simple self-interaction correction to random-phase-approximation-like correlation energies. Physical Review A, 2019, 100, .	1.0	13
77	Implementation of the Many-Pair Expansion for Systematically Improving Density Functional Calculations of Molecules. Journal of Chemical Theory and Computation, 2019, 15, 1089-1101.	2.3	5
78	TDDFT+U : A critical assessment of the Hubbard U correction to exchange-correlation kernels and potentials. Physical Review B, 2019, 99, .	1.1	8
79	Stretched or noded orbital densities and self-interaction correction in density functional theory. Journal of Chemical Physics, 2019, 150, 174102.	1.2	46
80	Fermi-Löwdin orbital self-interaction correction using the strongly constrained and appropriately normed meta-GGA functional. Journal of Chemical Physics, 2019, 151, 154105.	1.2	38
81	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. Journal of Chemical Physics, 2019, 151, 214108.	1.2	56
82	The Fermi-Löwdin self-interaction correction for ionization energies of organic molecules. Journal of Chemical Physics, 2020, 153, 184303.	1.2	12
83	Application of Self-Interaction Corrected Density Functional Theory to Early, Middle, and Late Transition States. Journal of Physical Chemistry A, 2020, 124, 8223-8234.	1.1	12
84	PyFLOSIC: Python-based Fermi-Löwdin orbital self-interaction correction. Journal of Chemical Physics, 2020, 153, 084104.	1.2	17
85	First-principles Hubbard U and Hund's J corrected approximate density functional theory predicts an accurate fundamental gap in rutile and anatase TiO_2 .	1.1	31
86	Improvements in the orbitalwise scaling down of Perdew-Zunger self-interaction correction in many-electron regions. Journal of Chemical Physics, 2020, 152, 174112.	1.2	23
87	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. II. Gauge consistency of the energy density at three levels of approximation. Journal of Chemical Physics, 2020, 152, 214109.	1.2	23
88	Piecewise linearity, freedom from self-interaction, and a Coulomb asymptotic potential: three related yet inequivalent properties of the exact density functional. Physical Chemistry Chemical Physics, 2020, 22, 16467-16481.	1.3	37
89	Fractional occupation numbers and self-interaction correction scaling methods with the Fermi-Löwdin orbital self-interaction correction approach. Journal of Computational Chemistry, 2020, 41, 1200-1208.	1.5	13
90	Asymptotic Behavior of the Exchange-Correlation Energy Density and the Kohn-Sham Potential in Density Functional Theory: Exact Results and Strategy for Approximations. Israel Journal of Chemistry, 2020, 60, 805-822.	1.0	14

#	ARTICLE	IF	CITATIONS
91	On the top rung of Jacob's ladder of density functional theory: Toward resolving the dilemma of <sc>SIE</sc> and <sc>NCE</sc>. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, .	6.2	25
92	Local self-interaction correction method with a simple scaling factor. Physical Chemistry Chemical Physics, 2021, 23, 2406-2418.	1.3	14
93	Density-related properties from self-interaction corrected density functional theory calculations. Journal of Chemical Physics, 2021, 154, 024102.	1.2	8
94	Replacing hybrid density functional theory: motivation and recent advances. Chemical Society Reviews, 2021, 50, 8470-8495.	18.7	80
95	Implementation of Perdew's Zunger self-interaction correction in real space using Fermi's Löwdin orbitals. Journal of Chemical Physics, 2021, 154, 084112.	1.2	7
96	Self-Interaction-Corrected Random Phase Approximation. Journal of Chemical Theory and Computation, 2021, 17, 2107-2115.	2.3	2
97	Self-interaction correction in water's ion clusters. Journal of Chemical Physics, 2021, 154, 094302.	1.2	16
98	Static dipole polarizabilities of polyacenes using self-interaction-corrected density functional approximations. Journal of Chemical Physics, 2021, 154, 114305.	1.2	12
99	Exploring and enhancing the accuracy of interior-scaled Perdew's Zunger self-interaction correction. Journal of Chemical Physics, 2021, 154, 094105.	1.2	12
100	Fermi-Löwdin-orbital self-interaction correction using the optimized-effective-potential method within the Krieger-Li-Iafrate approximation. Physical Review A, 2021, 103, .	1.0	14
101	N-dependent self-interaction corrections: Are they still appealing?. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	0
102	Initial Fermi orbital descriptors for FLOSIC calculations: The quick-FOD method. Chemical Physics Letters, 2021, 780, 138952.	1.2	4
103	How well do self-interaction corrections repair the overestimation of static polarizabilities in density functional calculations?. Physical Chemistry Chemical Physics, 2021, 23, 18678-18685.	1.3	14
104	Exact analytical ground state solution of 1D H ₂ ⁺ with soft Coulomb potential. Journal of Mathematical Chemistry, 2022, 60, 184-194.	0.7	3
105	Study of Self-Interaction Errors in Density Functional Calculations of Magnetic Exchange Coupling Constants Using Three Self-Interaction Correction Methods. Journal of Physical Chemistry A, 2022, 126, 1923-1935.	1.1	6
107	Molecular Orientation-Induced Second-Harmonic Generation: Deciphering Different Contributions Apart. Journal of Physical Chemistry A, 2022, 126, 3732-3738.	1.1	5
108	Delocalization error: The greatest outstanding challenge in density functional theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	6.2	43
109	Unification of Perdew's Zunger self-interaction correction, DFT+U, and Rung 3.5 density functionals. Journal of Chemical Physics, 2022, 157, .	1.2	3

#	ARTICLE	IF	CITATIONS
110	One-electron self-interaction error and its relationship to geometry and higher orbital occupation. Journal of Chemical Physics, 2023, 158, .	1.2	5
111	Density Matrix Implementation of the Fermiâ€™s Orbital Self-Interaction Correction Method. Journal of Physical Chemistry A, 2023, 127, 527-534.	1.1	2
112	Self-consistent implementation of locally scaled self-interaction-correction method. Journal of Chemical Physics, 2023, 158, .	1.2	6
113	Electronic structure and density functional theory. , 2023, , 3-35.		0
114	How Do Self-Interaction Errors Associated with Stretched Bonds Affect Barrier Height Predictions?. Journal of Physical Chemistry A, 2023, 127, 1750-1759.	1.1	3