

Stretched or noded orbital densities and self-interaction theory

Journal of Chemical Physics

150, 174102

DOI: [10.1063/1.5087065](https://doi.org/10.1063/1.5087065)

Citation Report

#	ARTICLE	IF	CITATIONS
1	Self-interaction-free electric dipole polarizabilities for atoms and their ions using the Fermi-Löwdin self-interaction correction. <i>Physical Review A</i> , 2019, 100, .	1.0	27
2	Interpretation and Automatic Generation of Fermi-Orbital Descriptors. <i>Journal of Computational Chemistry</i> , 2019, 40, 2843-2857.	1.5	21
3	The effect of self-interaction error on electrostatic dipoles calculated using density functional theory. <i>Journal of Chemical Physics</i> , 2019, 151, 174106.	1.2	29
4	Fermi-Löwdin orbital self-interaction correction using the strongly constrained and appropriately normed meta-GGA functional. <i>Journal of Chemical Physics</i> , 2019, 151, 154105.	1.2	38
5	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. <i>Journal of Chemical Physics</i> , 2019, 151, 214108.	1.2	56
6	Importance of self-interaction-error removal in density functional calculations on water cluster anions. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 3789-3799.	1.3	32
7	Symmetry-breaking polymorphous descriptions for correlated materials without interelectronic $\langle i U i \rangle$. <i>Physical Review B</i> , 2020, 102, .	1.1	48
8	The Fermi-Löwdin self-interaction correction for ionization energies of organic molecules. <i>Journal of Chemical Physics</i> , 2020, 153, 184303.	1.2	12
9	Assessing the effect of regularization on the molecular properties predicted by SCAN and self-interaction corrected SCAN meta-GGA. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 18060-18070.	1.3	6
10	Application of Self-Interaction Corrected Density Functional Theory to Early, Middle, and Late Transition States. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8223-8234.	1.1	12
11	PyFLOSIC: Python-based Fermi-Löwdin orbital self-interaction correction. <i>Journal of Chemical Physics</i> , 2020, 153, 084104.	1.2	17
12	Self-interaction error overbinds water clusters but cancels in structural energy differences. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 11283-11288.	3.3	57
13	Improvements in the orbitalwise scaling down of Perdew-Zunger self-interaction correction in many-electron regions. <i>Journal of Chemical Physics</i> , 2020, 152, 174112.	1.2	23
14	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. <i>Journal of Chemical Physics</i> , 2020, 152, 214109.	1.2	23
15	Local self-interaction correction method with a simple scaling factor. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2406-2418.	1.3	14
16	Replacing hybrid density functional theory: motivation and recent advances. <i>Chemical Society Reviews</i> , 2021, 50, 8470-8495.	18.7	80
17	Implementation of Perdew-Zunger self-interaction correction in real space using Fermi-Löwdin orbitals. <i>Journal of Chemical Physics</i> , 2021, 154, 084112.	1.2	7
18	Self-interaction correction in water-ion clusters. <i>Journal of Chemical Physics</i> , 2021, 154, 094302.	1.2	16

#	ARTICLE	IF	CITATIONS
19	Exploring and enhancing the accuracy of interior-scaled Perdew-Zunger self-interaction correction. <i>Journal of Chemical Physics</i> , 2021, 154, 094105.	1.2	12
20	Mn Dimer Can Be Described Accurately with Density Functional Calculations When Self-Interaction Correction Is Applied. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4240-4246.	2.1	7
21	Fermi-Landau orbital self-interaction correction using the optimized-effective-potential method within the Krieger-Li-lafrate approximation. <i>Physical Review A</i> , 2021, 103, .	1.0	14
22	Testing Self-Interaction Correction for Molecules in Solution. <i>Advanced Engineering Materials</i> , 0, , 2100572.	1.6	1
23	Benchmark test of a dispersion corrected revised Tao-Mo semilocal functional for thermochemistry, kinetics, and noncovalent interactions of molecules and solids. <i>Journal of Chemical Physics</i> , 2021, 155, 114102.	1.2	4
24	Nonlocal rung-3.5 correlation from the density matrix expansion: Flat-plane condition, thermochemistry, and kinetics. <i>Journal of Chemical Physics</i> , 2020, 153, 164116.	1.2	3
25	Insights from the density functional performance of water and water-solid interactions: SCAN in relation to other meta-GGAs. <i>Journal of Chemical Physics</i> , 2020, 153, 214116.	1.2	14
26	Local hybrid functionals augmented by a strong-correlation model. <i>Journal of Chemical Physics</i> , 2021, 155, 144101.	1.2	12
27	Study of self-interaction-errors in barrier heights using locally scaled and Perdew-Zunger self-interaction methods. <i>Journal of Chemical Physics</i> , 2022, 156, 014306.	1.2	12
28	Study of Self-Interaction Errors in Density Functional Calculations of Magnetic Exchange Coupling Constants Using Three Self-Interaction Correction Methods. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1923-1935.	1.1	6
29	Fermi-Landau orbital self-interaction correction of adsorption energies on transition metal ions. <i>Journal of Chemical Physics</i> , 2022, 156, 134102.	1.2	2
30	Data-driven and constrained optimization of semi-local exchange and nonlocal correlation functionals for materials and surface chemistry. <i>Journal of Computational Chemistry</i> , 2022, 43, 1104-1112.	1.5	3
31	Complex Fermi-Landau orbital self-interaction correction. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	5
32	Laplacian-level meta-generalized gradient approximation for solid and liquid metals. <i>Physical Review Materials</i> , 2022, 6, .	0.9	10
33	Effect of Molecular and Electronic Geometries on the Electronic Density in FLO-SIC. <i>Springer Proceedings in Physics</i> , 2022, , 167-186.	0.1	0
34	How good are recent density functionals for ground and excited states of one-electron systems?. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	6
35	Understanding Density-Driven Errors for Reaction Barrier Heights. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 532-543.	2.3	11
36	Symmetry Breaking with the SCAN Density Functional Describes Strong Correlation in the Singlet Carbon Dimer. <i>Journal of Physical Chemistry A</i> , 2023, 127, 384-389.	1.1	10

#	ARTICLE	IF	CITATIONS
37	Self-consistent implementation of locally scaled self-interaction-correction method. Journal of Chemical Physics, 2023, 158, .	1.2	6
38	Downward quantum learning from element 118: Automated generation of Fermiâ€“LÃƒwrdin orbitals for all atoms. Journal of Chemical Physics, 2023, 158, .	1.2	5
39	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
40	Modern Density Functionals Derived From First Principles. , 2024, , 69-77.		0