

Perdew-Zunger self-interaction correction: How wrong for large- Z atoms?

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Self-interaction-free electric dipole polarizabilities for atoms and their ions using the Fermi-LÅ¶wdin self-interaction correction. <i>Physical Review A</i> , 2019, 100, .	1.0	27
2	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
3	Stretched or noded orbital densities and self-interaction correction in density functional theory. <i>Journal of Chemical Physics</i> , 2019, 150, 174102.	1.2	46
4	Fermi-LÅ¶wdin 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	The Fermi-LÅ¶wdin self-interaction correction for ionization energies of organic molecules. <i>Journal of Chemical Physics</i> , 2020, 153, 184303.	1.2	12
7	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
8	Simple hydrogenic estimates for the exchange and correlation energies of atoms and atomic ions, with implications for density functional theory. <i>Journal of Chemical Physics</i> , 2020, 153, 074114.	1.2	10
9	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
10	PyFLOSIC: Python-based Fermi-LÅ¶wdin orbital self-interaction correction. <i>Journal of Chemical Physics</i> , 2020, 153, 084104.	1.2	17
11	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
12	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
13	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
14	First-principles modeling of binary layered topological insulators: Structural optimization and exchange-correlation functionals. <i>Physical Review B</i> , 2020, 101, .	1.1	11
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	Density-related properties from self-interaction corrected density functional theory calculations. <i>Journal of Chemical Physics</i> , 2021, 154, 024102.	1.2	8
17	Self-interaction correction in water-ion clusters. <i>Journal of Chemical Physics</i> , 2021, 154, 094302.	1.2	16
18	Static dipole polarizabilities of polyacenes using self-interaction-corrected density functional approximations. <i>Journal of Chemical Physics</i> , 2021, 154, 114305.	1.2	12

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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	First-principles calculations to investigate elastic, electronic and thermophysical properties of the Dy ₂ Bi ₂ Fe ₄ O ₁₂ ferromagnetic semiconductor. <i>Semiconductor Science and Technology</i> , 2021, 36, 095015.	1.0	1
21	How well do self-interaction corrections repair the overestimation of static polarizabilities in density functional calculations?. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18678-18685.	1.3	14
22	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
23	An account of chronological computational investigations to ascertain the role of p π -p π bonding in influencing the Lewis acidity of BX ₃ (X = F, Cl, Br and I): Evolution of novel parameters and relegation of π -type back bonding concept. <i>Coordination Chemistry Reviews</i> , 2022, 463, 214519.	9.5	3
24	Delocalization error: The greatest outstanding challenge in density-functional theory. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2023, 13, .	6.2	43
25	Laplacian-level meta-generalized gradient approximation for solid and liquid metals. <i>Physical Review Materials</i> , 2022, 6, .	0.9	10
26	Unification of Perdew-Zunger self-interaction correction, DFT+U, and Rung 3.5 density functionals. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	3
27	The Predictive Power of Exact Constraints and Appropriate Norms in Density Functional Theory. <i>Annual Review of Physical Chemistry</i> , 2023, 74, 193-218.	4.8	22
28	Self-consistent implementation of locally scaled self-interaction-correction method. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	6
29	Downward quantum learning from element 118: Automated generation of Fermi-Landau orbitals for all atoms. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	5
30	How Do Self-Interaction Errors Associated with Stretched Bonds Affect Barrier Height Predictions?. <i>Journal of Physical Chemistry A</i> , 2023, 127, 1750-1759.	1.1	3
31	Modern Density Functionals Derived From First Principles. , 2024, , 69-77.		0