

A step in the direction of resolving the paradox of Perde correction

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Citation Report

#	ARTICLE	IF	CITATIONS
1	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
2	The Fermi δ self-interaction correction for ionization energies of organic molecules. <i>Journal of Chemical Physics</i> , 2020, 153, 184303.	1.2	12
3	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
4	Study of self-interaction errors in density functional predictions of dipole polarizabilities and ionization energies of water clusters using Perdew δ Zunger and locally scaled self-interaction corrected methods. <i>Journal of Chemical Physics</i> , 2020, 153, 164304.	1.2	21
5	Accurate and Numerically Efficient r^2 SCAN Meta-Generalized Gradient Approximation. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 8208-8215.	2.1	335
6	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
7	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
8	PyFLOSIC: Python-based Fermi δ orbital self-interaction correction. <i>Journal of Chemical Physics</i> , 2020, 153, 084104.	1.2	17
9	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
10	Improvements in the orbitalwise scaling down of Perdew δ Zunger self-interaction correction in many-electron regions. <i>Journal of Chemical Physics</i> , 2020, 152, 174112.	1.2	23
11	A step in the direction of resolving the paradox of Perdew δ 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
12	Piecewise linearity, freedom from self-interaction, and a Coulomb asymptotic potential: three related yet inequivalent properties of the exact density functional. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16467-16481.	1.3	37
13	Local self-interaction correction method with a simple scaling factor. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2406-2418.	1.3	14
14	Density-related properties from self-interaction corrected density functional theory calculations. <i>Journal of Chemical Physics</i> , 2021, 154, 024102.	1.2	8
15	Replacing hybrid density functional theory: motivation and recent advances. <i>Chemical Society Reviews</i> , 2021, 50, 8470-8495.	18.7	80
16	What Types of Chemical Problems Benefit from Density-Corrected DFT? A Probe Using an Extensive and Chemically Diverse Test Suite. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1368-1379.	2.3	45
17	Implementation of Perdew δ Zunger self-interaction correction in real space using Fermi δ orbitals. <i>Journal of Chemical Physics</i> , 2021, 154, 084112.	1.2	7
18	Self-interaction correction in water δ ion clusters. <i>Journal of Chemical Physics</i> , 2021, 154, 094302.	1.2	16

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19	Static dipole polarizabilities of polyacenes using self-interaction-corrected density functional approximations. <i>Journal of Chemical Physics</i> , 2021, 154, 114305.	1.2	12
20	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
21	Fermi-Löwdin-orbital self-interaction correction using the optimized-effective-potential method within the Krieger-Li-Iafate 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	Developing Efficient Suzuki Cross-Coupling Catalysts by Doping Palladium Clusters with Silver. <i>ACS Catalysis</i> , 2021, 11, 11459-11468.	5.5	9
24	Density functionals with full nonlocal exchange, nonlocal $r_s^{-3.5}$ correlation, and $D3$ dispersion: Combined accuracy for general main-group thermochemistry, kinetics, and noncovalent interactions. <i>Journal of Computational Chemistry</i> , 2021, 42, 1974-1981.	1.5	2
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27	Initial Fermi orbital descriptors for FLOSIC calculations: The quick-FOD method. <i>Chemical Physics Letters</i> , 2021, 780, 138952.	1.2	4
28	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
29	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
30	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
31	First-principles wave-vector- and frequency-dependent exchange-correlation kernel for jellium at all densities. <i>Physical Review B</i> , 2022, 105, .	1.1	7
32	Density Functional Theory for Transition Metal Catalysis. , 2024, , 562-585.		0
33	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
34	First-principles derivation and properties of density-functional average-atom models. <i>Physical Review Research</i> , 2022, 4, .	1.3	10
35	Systematically Improvable Generalization of Self-Interaction Corrected Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 5698-5702.	2.1	5
36	Delocalization error: The greatest outstanding challenge in density-functional theory. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2023, 13, .	6.2	43

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37	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
38	Mean Value Ensemble Hubbard-U Correction for Spin-Crossover Molecules. Journal of Physical Chemistry Letters, 2022, 13, 12049-12054.	2.1	3
39	Understanding Density-Driven Errors for Reaction Barrier Heights. Journal of Chemical Theory and Computation, 2023, 19, 532-543.	2.3	11
40	Spin-crossover complexes: Self-interaction correction vs density correction. Journal of Chemical Physics, 2023, 158, .	1.2	4
41	Density Matrix Implementation of the Fermi's Local Orbital Self-Interaction Correction Method. Journal of Physical Chemistry A, 2023, 127, 527-534.	1.1	2
42	Application of a Simple Density-Functional Approximation to Non-identical Fermions in One-dimensional Confinement. Brazilian Journal of Physics, 2023, 53, .	0.7	0
43	The Predictive Power of Exact Constraints and Appropriate Norms in Density Functional Theory. Annual Review of Physical Chemistry, 2023, 74, 193-218.	4.8	22
44	Self-consistent implementation of locally scaled self-interaction-correction method. Journal of Chemical Physics, 2023, 158, .	1.2	6
45	Spin-state gaps and self-interaction-corrected density functional approximations: Octahedral Fe(II) complexes as case study. Journal of Chemical Physics, 2023, 158, .	1.2	7
46	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