Inclusion of exact exchange for self-interaction corrected H3 density functional potential energy surface

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#	Paper	IF	Citations
60	Benchmark calculations of chemical reactions in density functional theory: Comparison of the accurate Kohn Sham solution with generalized gradient approximations for the H2+H and H2+H2 reactions. *Journal of Chemical Physics*, **1999**, 111, 4056-4067	3.9	68
59	Flexible geometry of methyl amine. *Vibrational Spectroscopy*, **2000**, 22, 127-141	2.1	2
58	The Hartree product and the description of local and global quantities in atomic systems: A study within Kohn Sham theory. *Journal of Chemical Physics*, **2000**, 112, 1150-1157	3.9	21
57	The optimized effective potential and the self-interaction correction in density functional theory: Application to molecules. *Journal of Chemical Physics*, **2000**, 112, 7880-7890	3.9	91
56	Comparison of the Accurate Kohn Sham Solution with the Generalized Gradient Approximations (GGAs) for the SN2 Reaction F- + CH3F -p FCH3 + F-: A Qualitative Rule To Predict Success or Failure of GGAs. *Journal of Physical Chemistry A*, **2000**, 104, 8558-8565	2.8	147
55	The Failure of Generalized Gradient Approximations (GGAs) and Meta-GGAs for the Two-Center Three-Electron Bonds in He2+, (H2O)2+, and (NH3)2+. *Journal of Physical Chemistry A*, **2001**, 105, 9211-9218	2.8	78
54	Curing difficult cases in magnetic properties prediction with self-interaction corrected density functional theory. *Journal of Chemical Physics*, **2001**, 115, 26-42	3.9	118
53	Improving difficult reaction barriers with self-interaction corrected density functional theory. *Journal of Chemical Physics*, **2002**, 116, 7806-7813	3.9	120
52	Rate-equilibrium relationships in hydride transfer reactions: the role of intrinsic barriers. *Journal of the American Chemical Society*, **2002**, 124, 4084-92	16.4	47
51	Electron correlation and the self-interaction error of density functional theory. *Molecular Physics*, **2002**, 100, 1771-1790	1.7	184
50	The role of the HOOO(-) anion in the ozonation of alcohols: large differences in the gas-phase and in the solution-phase mechanism. *Journal of the American Chemical Society*, **2003**, 125, 9395-402	16.4	23
49	The impact of the self-interaction error on the density functional theory description of dissociating radical cations: ionic and covalent dissociation limits. *Journal of Chemical Physics*, **2004**, 120, 524-39	3.9	128
48	Theoretical study of hydrogenation of thiouracils and their base pairs with adenine. *International Journal of Quantum Chemistry*, **2004**, 99, 841-853	2.1	7
47	Effect of the self-interaction error for three-electron bonds: On the development of new exchange-correlation functionals. *Physical Chemistry Chemical Physics*, **2004**, 6, 1096-1112	3.6	103
46	Performance of Density Functionals for Calculating Barrier Heights of Chemical Reactions Relevant to Astrophysics. *Journal of Physical Chemistry A*, **2004**, 108, 7621-7636	2.8	78
45	Improved Description of Chemical Barriers with Generalized Gradient Approximations (GGAs) and Meta-GGAs. *Journal of Physical Chemistry A*, **2004**, 108, 4459-4469	2.8	46
44	Effect of the Perdew-Zunger self-interaction correction on the thermochemical performance of approximate density functionals. *Journal of Chemical Physics*, **2004**, 121, 8187-93	3.9	134

43	Ionization potentials and electron affinities in the Perdew-Zunger self-interaction corrected density-functional theory. *Journal of Chemical Physics*, **2005**, 122, 184107	3.9	88
42	Quantifying the effects of the self-interaction error in DFT: when do the delocalized states appear?. *Journal of Chemical Physics*, **2005**, 122, 224103	3.9	205
41	Binding energy curves from nonempirical density functionals. I. Covalent bonds in closed-shell and radical molecules. *Journal of Physical Chemistry A*, **2005**, 109, 11006-14	2.8	53
40	Prescription for the design and selection of density functional approximations: more constraint satisfaction with fewer fits. *Journal of Chemical Physics*, **2005**, 123, 62201	3.9	658
39	Scaling down the Perdew-Zunger self-interaction correction in many-electron regions. *Journal of Chemical Physics*, **2006**, 124, 94108	3.9	108
38	Kinetics of triscarbonato uranyl reduction by aqueous ferrous iron: a theoretical study. *Journal of Physical Chemistry A*, **2006**, 110, 9691-701	2.8	34
37	Spurious fractional charge on dissociated atoms: pervasive and resilient self-interaction error of common density functionals. *Journal of Chemical Physics*, **2006**, 125, 194112	3.9	349
36	Density functionals that are one- and two- are not always many-electron self-interaction-free, as shown for H2+, He2+, LiH+, and Ne2+. *Journal of Chemical Physics*, **2007**, 126, 104102	3.9	248
35	Range separated hybrid density functional with long-range Hartree-Fock exchange applied to solids. *Journal of Chemical Physics*, **2007**, 127, 054101	3.9	86
34	A Review of Density Functional Theory Quantum Mechanics as Applied to Pharmaceutically Relevant Systems. *Current Computer-Aided Drug Design*, **2007**, 3, 290-296	1.4	17
33	One-parameter optimization of a nonempirical meta-generalized-gradient-approximation for the exchange-correlation energy. *Physical Review A*, **2007**, 76,	2.6	37
32	Second step of hydrolytic dehalogenation in haloalkane dehalogenase investigated by QM/MM methods. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 707-17	4.2	24
31	Orbital-dependent density functionals: Theory and applications. *Reviews of Modern Physics*, **2008**, 80, 3-60	40.5	941
30	Range separation and local hybridization in density functional theory. *Journal of Physical Chemistry A*, **2008**, 112, 12530-42	2.8	81
29	Theoretical investigation of the electronic asymmetry of the special pair cation radical in the photosynthetic type-II reaction center. *Journal of Physical Chemistry B*, **2008**, 112, 13923-33	3.4	25
28	Self-interaction correction and the optimized effective potential. *Journal of Chemical Physics*, **2008**, 129, 014110	3.9	68
27	Many-electron self-interaction and spin polarization errors in local hybrid density functionals. *Journal of Chemical Physics*, **2010**, 133, 134116	3.9	78
26	An Assessment of Density Functional Methods for Potential Energy Curves of Nonbonded Interactions: The XYG3 and B97-D Approximations. *Journal of Chemical Theory and Computation*, **2010**, 6, 727-34	6.4	86

25	How Well Can Kohn-Sham DFT Describe the HO2 + O3 Reaction?. *Journal of Chemical Theory and Computation*, **2010**, 6, 2751-61	6.4	20
24	Modeling Charge Resonance in Cationic Molecular Clusters: Combining DFT-Tight Binding with Configuration Interaction. *Journal of Chemical Theory and Computation*, **2011**, 7, 44-55	6.4	42
23	A DFT study of H-isomerisation in alkoxy-, alkylperoxy- and alkyl radicals: Some implications for radical chain reactions in polymer systems. *Polymer Degradation and Stability*, **2011**, 96, 660-669	4.7	7
22	Using complex degrees of freedom in the Kohn-Sham self-interaction correction. *Physical Review A*, **2012**, 85,	2.6	45
21	Extensions of DFTB to investigate molecular complexes and clusters. *Physica Status Solidi (B): Basic Research*, **2012**, 249, 245-258	1.3	29
20	Theoretical Toolkits for Inorganic and Bioinorganic Complexes: Their Applications and Insights. **2013**, 1-57		1
19	Surface Reaction of Acetylene with H-Terminated Silicon Surfaces. A Theoretical Study from Hybrid DFT-D2 Periodic Simulations. *Journal of Physical Chemistry C*, **2013**, 117, 15130-15138	3.8	6
18	Variational, Self-Consistent Implementation of the Perdew-Zunger Self-Interaction Correction with Complex Optimal Orbitals. *Journal of Chemical Theory and Computation*, **2014**, 10, 5324-37	6.4	59
17	Comparison of ab Initio, DFT, and Semiempirical QM/MM Approaches for Description of Catalytic Mechanism of Hairpin Ribozyme. *Journal of Chemical Theory and Computation*, **2014**, 10, 1608-22	6.4	48
16	Correlated Ab Initio and Density Functional Studies on H2 Activation by FeO(.). *Journal of Chemical Theory and Computation*, **2014**, 10, 3807-20	6.4	75
15	Accurate Diels-Alder reaction energies from efficient density functional calculations. *Journal of Chemical Theory and Computation*, **2015**, 11, 2879-88	6.4	17
14	Modelling potential photovoltaic absorbers Cu3MCh4(M = V, Nb, Ta; Ch = S, Se, Te) using density functional theory. *Journal of Physics Condensed Matter*, **2016**, 28, 175801	1.8	10
13	Assessing the potential of Mg-doped CrO_2 as a novel p-type transparent conducting oxide. *Journal of Physics Condensed Matter*, **2016**, 28, 125501	1.8	16
12	Mechanisms of Formation of H, HO, and Water and of Water Desorption in the Early Stages of Cellulose Pyrolysis. *Journal of Physical Chemistry C*, **2018**, 122, 12168-12176	3.8	10
11	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. *Journal of Chemical Physics*, **2019**, 151, 214108	3.9	34
10	The Fermi-Löwdin self-interaction correction for ionization energies of organic molecules. *Journal of Chemical Physics*, **2020**, 153, 184303	3.9	9
9	Improvements in the orbitalwise scaling down of Perdew-Zunger self-interaction correction in many-electron regions. *Journal of Chemical Physics*, **2020**, 152, 174112	3.9	17
8	Wood cellulose as a hydrogen storage material. *International Journal of Hydrogen Energy*, **2020**, 45, 14907-14914	7.1	3

7	Local self-interaction correction method with a simple scaling factor. *Physical Chemistry Chemical Physics*, **2021**, 23, 2406-2418	3.6	9
6	Implementation of Perdew-Zunger self-interaction correction in real space using Fermi-L□wdin orbitals. *Journal of Chemical Physics*, **2021**, 154, 084112	3.9	4
5	How well do self-interaction corrections repair the overestimation of static polarizabilities in density functional calculations?. *Physical Chemistry Chemical Physics*, **2021**, 23, 18678-18685	3.6	6
4	Density-Functional Theory in External Electric and Magnetic Fields. *Modern Aspects of Electrochemistry*, **2009**, 341-408		1
3	Density-functional theory models of Fe(iv)O reactivity in metal-organic frameworks: self-interaction error, spin delocalisation and the role of hybrid exchange. *Physical Chemistry Chemical Physics*, **2020**, 22, 12821-12830	3.6	5
2	Kohn□Sham LCAO Method for Periodic Systems. *Springer Series in Solid-state Sciences*, **2012**, 251-301	0.4	
1	Delocalization error: The greatest outstanding challenge in density-functional theory. *Wiley Interdisciplinary Reviews: Computational Molecular Science*,	7.9	6