

Energies of organic molecules and atoms in density fun

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Nonempirical Construction of Current-Density Functionals from Conventional Density-Functional Approximations. <i>Physical Review Letters</i> , 2005, 95, 196403.	2.9	61
2	Binding Energy Curves from Nonempirical Density Functionals. I. Covalent Bonds in Closed-Shell and Radical Molecules. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11006-11014.	1.1	57
3	Test of a nonempirical density functional: Short-range part of the van der Waals interaction in rare-gas dimers. <i>Journal of Chemical Physics</i> , 2005, 122, 114102.	1.2	103
4	Binding Energy Curves from Nonempirical Density Functionals II. van der Waals Bonds in Rare-Gas and Alkaline-Earth Diatomics. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11015-11021.	1.1	82
5	Prescription for the design and selection of density functional approximations: More constraint satisfaction with fewer fits. <i>Journal of Chemical Physics</i> , 2005, 123, 062201.	1.2	769
6	The performance of semilocal and hybrid density functionals in 3d transition-metal chemistry. <i>Journal of Chemical Physics</i> , 2006, 124, 044103.	1.2	528
7	Parametrization of Atomic Energies to Improve Small Basis Set Density Functional Thermochemistry. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1045-1049.	2.3	17
8	Scaling down the Perdew-Zunger self-interaction correction in many-electron regions. <i>Journal of Chemical Physics</i> , 2006, 124, 094108.	1.2	122
9	Assessing a new nonempirical density functional: Difficulties in treating π -conjugation effects. <i>Journal of Chemical Physics</i> , 2006, 124, 124112.	1.2	34
10	Comparison of SCC-DFTB and NDDO-Based Semiempirical Molecular Orbital Methods for Organic Molecules. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13551-13559.	1.1	131
11	Meta-generalized gradient approximation for the exchange-correlation hole with an application to the jellium surface energy. <i>Physical Review B</i> , 2006, 73, .	1.1	71
12	Semiempirical hybrid density functional with perturbative second-order correlation. <i>Journal of Chemical Physics</i> , 2006, 124, 034108.	1.2	2,729
13	Density Functional Study of Methyl Chemisorption on Polycyclic Aromatic Hydrocarbons. <i>ChemPhysChem</i> , 2006, 7, 1311-1321.	1.0	6
14	One-parameter optimization of a nonempirical meta-generalized-gradient-approximation for the exchange-correlation energy. <i>Physical Review A</i> , 2007, 76, .	1.0	37
15	Laplacian-level density functionals for the kinetic energy density and exchange-correlation energy. <i>Physical Review B</i> , 2007, 75, .	1.1	120
16	Diminished gradient dependence of density functionals: Constraint satisfaction and self-interaction correction. <i>Journal of Chemical Physics</i> , 2007, 126, 244107.	1.2	26
17	Meta-generalized gradient approximation: non-empirical construction and performance of a density functional. <i>Philosophical Magazine</i> , 2007, 87, 1071-1084.	0.7	11
18	On Calculating a Polymer's Enthalpy of Formation with Quantum Chemical Methods. <i>Journal of Physical Chemistry B</i> , 2007, 111, 13869-13872.	1.2	8

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19	Application of the Computationally Efficient Self-Consistent-Charge Density-Functional Tight-Binding Method to Magnesium-Containing Molecules. Journal of Physical Chemistry A, 2007, 111, 5743-5750.	1.1	15
20	Restoring the Density-Gradient Expansion for Exchange in Solids and Surfaces. Physical Review Letters, 2008, 100, 136406.	2.9	8,139
21	Performance of B3LYP Density Functional Methods for a Large Set of Organic Molecules. Journal of Chemical Theory and Computation, 2008, 4, 297-306.	2.3	931
22	Enhanced Enthalpies of Formation from Density Functional Theory through Molecular Reference States. Journal of Physical Chemistry A, 2008, 112, 13706-13711.	1.1	6
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24	Polyfunctional Methodology for Improved DFT Thermochemical Predictions. Journal of Physical Chemistry A, 2008, 112, 10624-10634.	1.1	1
25	Absorption Spectra of Blue-Light-Emitting Oligoquinolines from Time-Dependent Density Functional Theory. Journal of Physical Chemistry B, 2008, 112, 13701-13710.	1.2	10
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27	Improved Description of Stereoelectronic Effects in Hydrocarbons Using Semilocal Density Functional Theory. Journal of Chemical Theory and Computation, 2008, 4, 888-891.	2.3	63
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30	“Mindless” DFT Benchmarking. Journal of Chemical Theory and Computation, 2009, 5, 993-1003.	2.3	215
31	Evaluation of Density Functionals and Basis Sets for Carbohydrates. Journal of Chemical Theory and Computation, 2009, 5, 679-692.	2.3	183
32	Unified Inter- and Intramolecular Dispersion Correction Formula for Generalized Gradient Approximation Density Functional Theory. Journal of Chemical Theory and Computation, 2009, 5, 2950-2958.	2.3	76
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37	Doubly hybrid density functional for accurate description of thermochemistry, thermochemical kinetics and nonbonded interactions. International Reviews in Physical Chemistry, 2011, 30, 115-160.	0.9	116

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38	Theoretical study of substituent and solvent effects on the thermodynamics for cis/trans isomerization and intramolecular rearrangements of 2,2-diphenyl-1,3-butadiene. <i>Structural Chemistry</i> , 2011, 22, 615-625.	1.0	5
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40	A meta-GGA Made Free of the Order of Limits Anomaly. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2078-2087.	2.3	49
41	N ₂ H and N ₂ Cl homolytic bond dissociation energies and radical stabilization energies: An assessment of theoretical procedures through comparison with benchmark-quality W2w data. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 1862-1878.	1.0	46
42	The calculation of active Raman modes of α -quartz crystal via density functional theory based on B3LYP Hamiltonian in 6-311+G(2d) basis set. <i>Pramana - Journal of Physics</i> , 2012, 78, 803-810.	0.9	5
43	Performance of meta-GGA Functionals on General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 355-363.	2.3	68
44	Parametrization and Benchmark of DFTB3 for Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 338-354.	2.3	743
45	Assessment of Density Functional Theory for Thermochemical Approaches Based on Bond Separation Reactions. <i>Journal of Physical Chemistry A</i> , 2013, 117, 228-243.	1.1	16
46	The calculation of the energies of phonon normal modes in the alpha-quartz crystal by analyzing the change of forces on atoms in the hydrogen-passivated small cluster of H16Si7O6. <i>Optik</i> , 2014, 125, 224-227.	1.4	1
47	A comparative DFT study on the differences between normal modes of polyethylene and polyethylene glycol via B3LYP Hamiltonian and the Hartree-Fock method in multiple bases. <i>Optik</i> , 2014, 125, 228-231.	1.4	8
48	Strongly Constrained and Appropriately Normed Semilocal Density Functional. <i>Physical Review Letters</i> , 2015, 115, 036402.	2.9	2,273
49	Construction and Application of a New Dual-Hybrid Random Phase Approximation. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4615-4626.	2.3	54
50	Why Density Functionals Should Not Be Judged Primarily by Atomization Energies. <i>Periodica Polytechnica: Chemical Engineering</i> , 2016, 60, 2-7.	0.5	18
51	Performance of a nonempirical density functional on molecules and hydrogen-bonded complexes. <i>Journal of Chemical Physics</i> , 2016, 145, 234306.	1.2	25
52	Semilocal density functionals and constraint satisfaction. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 847-851.	1.0	65
53	The two pillars: density and spin-density functional theories. <i>Molecular Physics</i> , 2016, 114, 928-931.	0.8	6
54	Performance of a nonempirical exchange functional from density matrix expansion: comparative study with different correlations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 21707-21713.	1.3	20
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57	Crystal structure and DFT studies of (E)-1-(4-fluorophenyl)-3-(1H-indol-1-yl)-4-styrylazetid-2-one. Journal of Molecular Structure, 2019, 1187, 50-58.	1.8	9
58	Response to "Comment on "Regularized SCAN functional" [J. Chem. Phys. 151, 207101 (2019)]. Journal of Chemical Physics, 2019, 151, 207102.	1.2	10
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61	Density Functional Theory for Electrocatalysis. Energy and Environmental Materials, 2022, 5, 157-185.	7.3	95
62	ReaxFF molecular dynamics study on pyrolysis of bicyclic compounds for aviation fuel. Fuel, 2021, 297, 120724.	3.4	36
63	The Connectivity Matrix: A Toolbox for Monitoring Bonded Atoms and Bonds. Journal of Physical Chemistry A, 2020, 124, 1076-1086.	1.1	4
64	Improving the Accuracy of Composite Methods: A G4MP2 Method with G4-like Accuracy and Implications for Machine Learning. Journal of Physical Chemistry A, 2022, 126, 4528-4536.	1.1	3