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Condition on the Kohn-Sham kinetic energy and modern parametrization of the Thomas-Fermi density

DOI: 10.1063/1.3059783

Journal of Chemical Physics, 2009, 130, 034107.

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**Version:** 2024-04-28

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#	Paper	IF	Citations
58	Kinetic energy density functionals from the Airy gas with an application to the atomization kinetic energies of molecules. <i>Physical Review B</i> , <b>2009</b> , 79,	3.3	24
57	Conditions on the Kohn-Sham kinetic energy and associated density. <i>International Journal of Quantum Chemistry</i> , <b>2009</b> , 109, 2943-2952	2.1	23
56	Non-empirical derivation of the parameter in the B88 exchange functional. <i>Canadian Journal of Chemistry</i> , <b>2009</b> , 87, 1485-1491	0.9	72
55	Leading corrections to local approximations. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	25
54	Generalized Gradient Approximations of the Noninteracting Kinetic Energy from the Semiclassical Atom Theory: Rationalization of the Accuracy of the Frozen Density Embedding Theory for Nonbonded Interactions. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 2439-51	6.4	68
53	Two-Dimensional Scan of the Performance of Generalized Gradient Approximations with Perdew-Burke-Ernzerhof-Like Enhancement Factor. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 3548-59	6.4	46
52	Semiclassical neutral atom as a reference system in density functional theory. <i>Physical Review Letters</i> , <b>2011</b> , 106, 186406	7.4	101
51	Spin-dependent gradient correction for more accurate atomization energies of molecules. <i>Journal of Chemical Physics</i> , <b>2012</b> , 137, 194105	3.9	21
50	Finding density functionals with machine learning. <i>Physical Review Letters</i> , <b>2012</b> , 108, 253002	7.4	400
49	A meta-GGA Made Free of the Order of Limits Anomaly. <i>Journal of Chemical Theory and Computation</i> , <b>2012</b> , 8, 2078-87	6.4	44
48	The reduced density gradient in atoms. <i>International Journal of Quantum Chemistry</i> , <b>2012</b> , 112, 3594-3598	8.1	18
47	Testing the broad applicability of the PBEint GGA functional and its one-parameter hybrid form. <i>International Journal of Quantum Chemistry</i> , <b>2013</b> , 113, 673-682	2.1	29
46	Theory of variational calculation with a scaling correct moment functional to solve the electronic Schrödinger equation directly for ground state one-electron density and electronic energy. <i>International Journal of Quantum Chemistry</i> , <b>2013</b> , 113, 1479-1492	2.1	3
45	Relevance of coordinate and particle-number scaling in density-functional theory. <i>Physical Review A</i> , <b>2013</b> , 87,	2.6	34
44	Electron avoidance: A nonlocal radius for strong correlation. <i>Physical Review A</i> , <b>2014</b> , 90,	2.6	21
43	Quantum oscillations in the kinetic energy density: Gradient corrections from the Airy gas. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	18
42	Subsystem density-functional theory. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2014</b> , 4, 325-362	7.9	235

41	Generalized Gradient Approximation Correlation Energy Functionals Based on the Uniform Electron Gas with Gap Model. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 2016-26	6.4	17
40	Laplacian-Level Kinetic Energy Approximations Based on the Fourth-Order Gradient Expansion: Global Assessment and Application to the Subsystem Formulation of Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 164-79	6.4	52
39	Communication: Testing and using the Lewin-Lieb bounds in density functional theory. <i>Journal of Chemical Physics</i> , <b>2014</b> , 141, 241105	3.9	9
38	Correction to kinetic energy density functional using exactly solvable model. <i>Physica Scripta</i> , <b>2015</b> , 90, 125401	2.6	3
37	Global hybrids from the semiclassical atom theory satisfying the local density linear response. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 122-31	6.4	20
36	Subsystem density functional theory with meta-generalized gradient approximation exchange-correlation functionals. <i>Journal of Chemical Physics</i> , <b>2015</b> , 142, 154121	3.9	21
35	Kinetic and Exchange Energy Densities near the Nucleus. <i>Computation</i> , <b>2016</b> , 4, 19	2.2	18
34	Study of some simple approximations to the non-interacting kinetic energy functional. <i>International Journal of Quantum Chemistry</i> , <b>2016</b> , 116, 1313-1321	2.1	18
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32	Locality of correlation in density functional theory. <i>Journal of Chemical Physics</i> , <b>2016</b> , 145, 054112	3.9	24
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30	Leading gradient correction to the kinetic energy for two-dimensional fermion gases. <i>Physical Review A</i> , <b>2016</b> , 93,	2.6	4
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28	Functional constructions with specified functional derivatives. <i>Theoretical Chemistry Accounts</i> , <b>2016</b> , 135, 1	1.9	3
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26	Kinetic Energy of Hydrocarbons as a Function of Electron Density and Convolutional Neural Networks. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 1139-47	6.4	81
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24	Jellium-with-gap model applied to semilocal kinetic functionals. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	21

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22	Leading corrections to local approximations. II. The case with turning points. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	9
21	Modified Fourth-Order Kinetic Energy Gradient Expansion with Hartree Potential-Dependent Coefficients. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 4228-4239	6.4	24
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19	Orbital-free density functional theory for materials research. <i>Journal of Materials Research</i> , <b>2018</b> , 33, 777-795	2.5	68
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17	A fragment-based approximation of the Pauli kinetic energy. <i>Theoretical Chemistry Accounts</i> , <b>2018</b> , 137, 1	1.9	7
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14	The first order atomic fragment approach-An orbital-free implementation of density functional theory. <i>Journal of Chemical Physics</i> , <b>2019</b> , 151, 024109	3.9	11
13	An alternative derivation of orbital-free density functional theory. <i>Journal of Chemical Physics</i> , <b>2019</b> , 150, 204109	3.9	2
12	A study of the basis set dependence of the bifunctional expression of the non-interacting kinetic energy for atomic systems. <i>Computational and Theoretical Chemistry</i> , <b>2019</b> , 1155, 56-60	2	4
11	Performance of Semilocal Kinetic Energy Functionals for Orbital-Free Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 3044-3055	6.4	18
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4	Approximate Analytical Solutions for the Euler Equation for Second-Row Homonuclear Dimers. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 6832-6840	6.4	1
3	Analysis of atomic Pauli potentials and their large-Z limit. <i>Journal of Chemical Physics</i> , <b>2021</b> , 155, 134112, 3.9		1
2	Gradient Expansions for the Large-Coupling Strength Limit of the Müller-Plesset Adiabatic Connection.. <i>Journal of Chemical Theory and Computation</i> , <b>2022</b> ,	6.4	0
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