

Matthias Ernzerhof

List of Publications by Year in descending order

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69
papers

194,782
citations

230014

27
h-index

120465

65
g-index

69
all docs

69
docs citations

69
times ranked

109622
citing authors

#	ARTICLE	IF	CITATIONS
1	Generalized Gradient Approximation Made Simple. <i>Physical Review Letters</i> , 1996, 77, 3865-3868.	2.9	157,044
2	Hybrid functionals based on a screened Coulomb potential. <i>Journal of Chemical Physics</i> , 2003, 118, 8207-8215.	1.2	14,063
3	Generalized Gradient Approximation Made Simple [Phys. Rev. Lett. 77, 3865 (1996)]. <i>Physical Review Letters</i> , 1997, 78, 1396-1396.	2.9	12,087
4	Rationale for mixing exact exchange with density functional approximations. <i>Journal of Chemical Physics</i> , 1996, 105, 9982-9985.	1.2	4,987
5	Assessment of the Perdew-Burke-Ernzerhof exchange-correlation functional. <i>Journal of Chemical Physics</i> , 1999, 110, 5029-5036.	1.2	3,841
6	Generalized gradient approximation to the angle- and system-averaged exchange hole. <i>Journal of Chemical Physics</i> , 1998, 109, 3313-3320.	1.2	425
7	Coupling-constant dependence of atomization energies. <i>International Journal of Quantum Chemistry</i> , 1997, 64, 285-295.	1.0	174
8	Why semilocal functionals work: Accuracy of the on-top pair density and importance of system averaging. <i>Journal of Chemical Physics</i> , 1998, 109, 3760-3771.	1.2	167
9	Construction of the adiabatic connection. <i>Chemical Physics Letters</i> , 1996, 263, 499-506.	1.2	164
10	Distributions and averages of electron density parameters: Explaining the effects of gradient corrections. <i>Journal of Chemical Physics</i> , 1997, 106, 10184-10193.	1.2	144
11	Current-dependent extension of the Perdew-Burke-Ernzerhof exchange-correlation functional. <i>Journal of Chemical Physics</i> , 2004, 120, 2105-2109.	1.2	142
12	Why the generalized gradient approximation works and how to go beyond it. <i>International Journal of Quantum Chemistry</i> , 1997, 61, 287-293.	1.0	126
13	The meta-GGA functional: Thermochemistry with a kinetic energy density dependent exchange-correlation functional. <i>Journal of Chemical Physics</i> , 2000, 112, 2643-2649.	1.2	114
14	On-top pair-density interpretation of spin density functional theory, with applications to magnetism. <i>International Journal of Quantum Chemistry</i> , 1997, 61, 197-205.	1.0	97
15	Nonlocality of the density functional for exchange and correlation: Physical origins and chemical consequences. <i>Journal of Chemical Physics</i> , 1998, 108, 1522-1531.	1.2	88
16	Kinetic energy density dependent approximations to the exchange energy. <i>Journal of Chemical Physics</i> , 1999, 111, 911-915.	1.2	83
17	Source and sink potentials for the description of open systems with a stationary current passing through. <i>Journal of Chemical Physics</i> , 2007, 126, 144104.	1.2	76
18	Electron Transmission through Aromatic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1291-1297.	2.3	74

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19	Side-chain effects in molecular electronic devices. <i>Journal of Chemical Physics</i> , 2005, 123, 134704.	1.2	63
20	Mechanism of a molecular electronic photoswitch. <i>Physical Review B</i> , 2005, 72, .	1.1	57
21	Local and Gradient-Corrected Density Functionals. <i>ACS Symposium Series</i> , 1996, , 453-462.	0.5	56
22	Long-range asymptotic behavior of ground-state wave functions, one-electron matrices, and pair densities. <i>Journal of Chemical Physics</i> , 1996, 105, 2798-2803.	1.2	51
23	A simple model of molecular electronic devices and its analytical solution. <i>Journal of Chemical Physics</i> , 2007, 127, 204709.	1.2	45
24	Calculating the Lifetimes of Metastable States with Complex Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 1916-1920.	2.1	41
25	Communication: A non-empirical correlation factor model for the exchange-correlation energy. <i>Journal of Chemical Physics</i> , 2014, 141, 111102.	1.2	34
26	Design of exchange-correlation functionals through the correlation factor approach. <i>Journal of Chemical Physics</i> , 2015, 143, 144102.	1.2	30
27	Zero-voltage conductance of short gold nanowires. <i>Journal of Chemical Physics</i> , 2004, 120, 4921-4926.	1.2	27
28	Density functional theory of complex transition densities. <i>Journal of Chemical Physics</i> , 2006, 125, 124104.	1.2	27
29	Generalized-gradient exchange-correlation hole obtained from a correlation factor ansatz. <i>Journal of Chemical Physics</i> , 2008, 128, 234104.	1.2	27
30	The shell model for the exchange-correlation hole in the strong-correlation limit. <i>Journal of Chemical Physics</i> , 2016, 145, 124104.	1.2	27
31	Rhodium(^{II})-catalyzed C-H aminations using <i>N</i> -mesyloxycarbamates: reaction pathway and by-product formation. <i>Chemical Science</i> , 2019, 10, 718-729.	3.7	26
32	Construction of exchange-correlation functionals through interpolation between the non-interacting and the strong-correlation limit. <i>Journal of Chemical Physics</i> , 2015, 143, 124103.	1.2	23
33	The Zero-Voltage Conductance of Nanographenes: Simple Rules and Quantitative Estimates. <i>Journal of Physical Chemistry C</i> , 2013, 117, 7870-7884.	1.5	22
34	Simple orbital theory for the molecular electrician. <i>Journal of Chemical Physics</i> , 2011, 135, 014104.	1.2	18
35	Molecular conductance obtained in terms of orbital densities and response functions. <i>Journal of Chemical Physics</i> , 2009, 130, 184704.	1.2	17
36	Approximating the exchange energy through the nonempirical exchange-factor approach. <i>Physical Review A</i> , 2014, 90, .	1.0	16

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37	Correlation effects in molecular conductors. <i>Journal of Chemical Physics</i> , 2011, 134, 174101.	1.2	15
38	Open-system Kohn-Sham density functional theory. <i>Journal of Chemical Physics</i> , 2012, 136, 094105.	1.2	15
39	Current transport through molecular electronic devices. <i>Journal of Chemical Physics</i> , 2003, 119, 4134-4140.	1.2	14
40	Perspective on "Inhomogeneous electron gas". <i>Theoretical Chemistry Accounts</i> , 2000, 103, 259-262.	0.5	13
41	A density functional method for the calculation of the zero-voltage conductance of molecular electronic devices. <i>International Journal of Quantum Chemistry</i> , 2005, 101, 557-563.	1.0	13
42	Approximate density functionals applied to molecular quantum dots. <i>Journal of Chemical Physics</i> , 2005, 122, 154705.	1.2	13
43	Modeling of molecular photocells: Application to two-level photovoltaic system with electron-hole interaction. <i>Journal of Chemical Physics</i> , 2016, 145, 124116.	1.2	13
44	A Mechanistic Study of the Stereochemical Outcomes of Rhodium-Catalysed Styrene Aziridinations. <i>Advanced Synthesis and Catalysis</i> , 2020, 362, 384-397.	2.1	13
45	Functionals of quantities other than the electron density: Approximations to the exchange energy. <i>Journal of Chemical Physics</i> , 2002, 116, 3980-3984.	1.2	12
46	Simple model of a coherent molecular photocell. <i>Journal of Chemical Physics</i> , 2016, 144, 134102.	1.2	12
47	Surface Plasmon Polariton-Controlled Molecular Switch. <i>Journal of Physical Chemistry C</i> , 2018, 122, 20083-20089.	1.5	12
48	Bond dissociation and correlation effects in molecular electronic devices. <i>Journal of Chemical Physics</i> , 2008, 129, 194901.	1.2	11
49	The impact of long-range electron-hole interaction on the charge separation yield of molecular photocells. <i>Journal of Chemical Physics</i> , 2017, 146, 034103.	1.2	10
50	The correlation factor model for the exchange-correlation energy and its application to transition metal compounds. <i>Journal of Chemical Physics</i> , 2019, 150, 084107.	1.2	10
51	Extension of the source-sink potential (SSP) approach to multichannel quantum transport. <i>Journal of Chemical Physics</i> , 2012, 137, 174112.	1.2	9
52	Constructing and representing exchange-correlation holes through artificial neural networks. <i>Journal of Chemical Physics</i> , 2021, 155, 174121.	1.2	9
53	Conjugated Molecules Described by a One-Dimensional Dirac Equation. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1818-1824.	2.3	8
54	Construction of self-interaction-corrected exchange-correlation functionals within the correlation factor approach. <i>Journal of Chemical Physics</i> , 2019, 151, 194102.	1.2	8

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55	Non-Hermitian quantum mechanics and exceptional points in molecular electronics. Journal of Chemical Physics, 2020, 152, 244119.	1.2	8
56	Rhodium-Catalyzed Sulfimidation Reactions: A Computational Study. Organometallics, 2021, 40, 3267-3275.	1.1	8
57	Taylor-series expansion of density functionals. Physical Review A, 1994, 50, 4593-4607.	1.0	7
58	The slowly-varying noninteracting electron gas in terms of its kinetic energy density. Journal of Chemical Physics, 2000, 112, 5270-5274.	1.2	7
59	Functionals of the square kinetic energy density. Journal of Chemical Physics, 2002, 117, 3074-3080.	1.2	7
60	The correlation factor approach: Combining density functional and wave function theory. Journal of Chemical Physics, 2020, 152, 211101.	1.2	6
61	Why the generalized gradient approximation works and how to go beyond it. , 1997, 61, 287.		5
62	Coherent molecular transistor: Control through variation of the gate wave function. Journal of Chemical Physics, 2014, 140, 114708.	1.2	4
63	Fourth-order series expansion of the exchange hole. Physical Review A, 2017, 96, .	1.0	4
64	Coupling-constant dependence of atomization energies. , 1997, 64, 285.		4
65	On-top pair-density interpretation of spin density functional theory, with applications to magnetism. , 0, .		3
66	Coupling-constant dependence of atomization energies. International Journal of Quantum Chemistry, 1997, 64, 285-295.	1.0	3
67	Why Density-Gradient Corrections Improve Atomization Energies and Barrier Heights. Advances in Quantum Chemistry, 1998, 33, 1-9.	0.4	2
68	Extending the source-sink potential method to include electron-nucleus coupling. Journal of Chemical Physics, 2021, 155, 014110.	1.2	1
69	The factorization ansatz for non-local approximations to the exchange-correlation hole. Journal of Chemical Physics, 2022, 156, 184110.	1.2	0