Matthias Ernzerhof

List of Publications by Year
in descending order

69 papers	194,782 citations	201385 27 h-index	106150 65 g-index
69 all docs	69 docs citations	69 times ranked	96960 citing authors

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

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

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37	Correlation effects in molecular conductors. Journal of Chemical Physics, 2011, 134, 174101.	1.2	15
38	Open-system Kohn-Sham density functional theory. Journal of Chemical Physics, 2012, 136, 094105.	1.2	15
39	Current transport through molecular electronic devices. Journal of Chemical Physics, 2003, 119, 4134-4140.	1.2	14
40	Perspective on "Inhomogeneous electron gas". Theoretical Chemistry Accounts, 2000, 103, 259-262.	0.5	13
41	A density functional method for the calculation of the zero-voltage conductance of molecular electronic devices. International Journal of Quantum Chemistry, 2005, 101, 557-563.	1.0	13
42	Approximate density functionals applied to molecular quantum dots. Journal of Chemical Physics, 2005, 122, 154705.	1.2	13
43	Modeling of molecular photocells: Application to two-level photovoltaic system with electron-hole interaction. Journal of Chemical Physics, 2016, 145, 124116.	1.2	13
44	A Mechanistic Study of the Stereochemical Outcomes of Rhodiumâ€Catalysed Styrene Aziridinations. Advanced Synthesis and Catalysis, 2020, 362, 384-397.	2.1	13
45	Functionals of quantities other than the electron density: Approximations to the exchange energy. Journal of Chemical Physics, 2002, 116, 3980-3984.	1.2	12
46	Simple model of a coherent molecular photocell. Journal of Chemical Physics, 2016, 144, 134102.	1.2	12
47	Surface Plasmon Polariton-Controlled Molecular Switch. Journal of Physical Chemistry C, 2018, 122, 20083-20089.	1.5	12
48	Bond dissociation and correlation effects in molecular electronic devices. Journal of Chemical Physics, 2008, 129, 194901.	1.2	11
49	The impact of long-range electron-hole interaction on the charge separation yield of molecular photocells. Journal of Chemical Physics, 2017, 146, 034103.	1.2	10
50	The correlation factor model for the exchange-correlation energy and its application to transition metal compounds. Journal of Chemical Physics, 2019, 150, 084107.	1.2	10
51	Extension of the source-sink potential (SSP) approach to multichannel quantum transport. Journal of Chemical Physics, 2012, 137, 174112.	1.2	9
52	Constructing and representing exchangeâ€“correlation holes through artificial neural networks. Journal of Chemical Physics, 2021, 155, 174121.	1.2	9
53	Conjugated Molecules Described by a One-Dimensional Dirac Equation. Journal of Chemical Theory and Computation, 2010, 6, 1818-1824.	2.3	8
54	Construction of self-interaction-corrected exchange-correlation functionals within the correlation factor approach. Journal of Chemical Physics, 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	Couplingâ€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 sourceâ€“sink potential method to include electronâ€“nucleus coupling. Journal of Chemical Physics, 2021, 155, 014110.	1.2	1
69	The factorization ansatz for non-local approximations to the exchangeâ€“correlation hole. Journal of Chemical Physics, 2022, 156, 184110.	1.2	0