

Kieron Burke

List of Publications by Year in descending order

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99795
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#	ARTICLE	IF	CITATIONS
1	Density-Corrected DFT Explained: Questions and Answers. Journal of Chemical Theory and Computation, 2022, 18, 817-827.	5.3	33
2	How Well Does Kohn-Sham Regularizer Work for Weakly Correlated Systems?. Journal of Physical Chemistry Letters, 2022, 13, 2540-2547.	4.6	6
3	Improving Results by Improving Densities: Density-Corrected Density Functional Theory. Journal of the American Chemical Society, 2022, 144, 6625-6639.	13.7	45
4	Correlation energy of the uniform electron gas determined by ground-state conditional probability density functional theory. Physical Review B, 2022, 105, .	3.2	2
5	Machine learning and density functional theory. Nature Reviews Physics, 2022, 4, 357-358.	26.6	37
6	Conditional probability density functional theory. Physical Review B, 2022, 105, .	3.2	4
7	Uncommonly accurate energies for the general quartic oscillator. International Journal of Quantum Chemistry, 2021, 121, e26554.	2.0	10
8	Density Sensitivity of Empirical Functionals. Journal of Physical Chemistry Letters, 2021, 12, 800-807.	4.6	29
9	Calculation and interpretation of classical turning surfaces in solids. Npj Computational Materials, 2021, 7, .	8.7	6
10	Learning to Approximate Density Functionals. Accounts of Chemical Research, 2021, 54, 818-826.	15.6	50
11	Explaining and Fixing DFT Failures for Torsional Barriers. Journal of Physical Chemistry Letters, 2021, 12, 2796-2804.	4.6	23
12	Bob Cave Memorial. Journal of Physical Chemistry A, 2021, 125, 4037-4038.	2.5	0
13	Response to comment. International Journal of Quantum Chemistry, 2021, 121, e26767.	2.0	0
14	Kohn-Sham Equations as Regularizer: Building Prior Knowledge into Machine-Learned Physics. Physical Review Letters, 2021, 126, 036401.	7.8	89
15	Exact and approximate energy sums in potential wells. Journal of Physics A: Mathematical and Theoretical, 2020, 53, 095203.	2.1	9
16	Quantum chemical accuracy from density functional approximations via machine learning. Nature Communications, 2020, 11, 5223.	12.8	187
17	Retrospective on a decade of machine learning for chemical discovery. Nature Communications, 2020, 11, 4895.	12.8	96
18	Measuring Density-Driven Errors Using Kohn-Sham Inversion. Journal of Chemical Theory and Computation, 2020, 16, 5014-5023.	5.3	28

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19	Challenges for large scale simulation: general discussion. Faraday Discussions, 2020, 224, 309-332.	3.2	2
20	New density-functional approximations and beyond: general discussion. Faraday Discussions, 2020, 224, 166-200.	3.2	1
21	Confirmation of the PPLB Derivative Discontinuity: Exact Chemical Potential at Finite Temperatures of a Model System. Journal of Chemical Theory and Computation, 2020, 16, 7225-7231.	5.3	5
22	New approaches to study excited states in density functional theory: general discussion. Faraday Discussions, 2020, 224, 483-508.	3.2	2
23	Quantifying and Understanding Errors in Molecular Geometries. Journal of Physical Chemistry Letters, 2020, 11, 9957-9964.	4.6	37
24	Simple hydrogenic estimates for the exchange and correlation energies of atoms and atomic ions, with implications for density functional theory. Journal of Chemical Physics, 2020, 153, 074114.	3.0	10
25	Deriving approximate functionals with asymptotics. Faraday Discussions, 2020, 224, 98-125.	3.2	3
26	MAP: An MP2 Accuracy Predictor for Weak Interactions from Adiabatic Connection Theory. Journal of Chemical Theory and Computation, 2020, 16, 4141-4149.	5.3	10
27	Leading correction to the local density approximation of the kinetic energy in one dimension. Journal of Chemical Physics, 2020, 152, 081102.	3.0	6
28	Bypassing the Energy Functional in Density Functional Theory: Direct Calculation of Electronic Energies from Conditional Probability Densities. Physical Review Letters, 2020, 125, 266401.	7.8	8
29	Recent Developments in Density Functional Approximations. , 2020, , 213-226.		3
30	Semiclassical quantization of truncated potentials. European Journal of Physics, 2019, 40, 065403.	0.6	6
31	Density Functional Analysis: The Theory of Density-Corrected DFT. Journal of Chemical Theory and Computation, 2019, 15, 6636-6646.	5.3	66
32	Halogen and Chalcogen Binding Dominated by Density-Driven Errors. Journal of Physical Chemistry Letters, 2019, 10, 295-301.	4.6	43
33	Benchmarks and Reliable DFT Results for Spin Gaps of Small Ligand Fe(II) Complexes. Journal of Chemical Theory and Computation, 2018, 14, 2304-2311.	5.3	71
34	Warming Up Density Functional Theory. , 2018, , 249-271.		15
35	Thermal stitching: Combining the advantages of different quantum fermion solvers. Physical Review B, 2018, 98, .	3.2	4
36	Accurate double excitations from ensemble density functional calculations. Journal of Chemical Physics, 2018, 149, 134103.	3.0	26

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37	Recent Developments in Density Functional Approximations. , 2018, , 1-14.		2
38	Quantifying Density Errors in DFT. Journal of Physical Chemistry Letters, 2018, 9, 6385-6392.	4.6	67
39	Fitting a round peg into a round hole: Asymptotically correcting the generalized gradient approximation for correlation. Journal of Chemical Physics, 2018, 149, 084116.	3.0	33
40	Guest Editorial: Special Topic on Data-Enabled Theoretical Chemistry. Journal of Chemical Physics, 2018, 148, 241401.	3.0	77
41	Linear response time-dependent density functional theory of the Hubbard dimer. European Physical Journal B, 2018, 91, 1.	1.5	33
42	Can exact conditions improve machine-learned density functionals?. Journal of Chemical Physics, 2018, 148, 241743.	3.0	39
43	Deriving uniform semiclassical approximations for one-dimensional fermionic systems. Journal of Chemical Physics, 2018, 148, 194103.	3.0	10
44	Understanding band gaps of solids in generalized Kohn-Sham theory. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2801-2806.	7.1	423
45	The Importance of Being Inconsistent. Annual Review of Physical Chemistry, 2017, 68, 555-581.	10.8	93
46	Bypassing the Kohn-Sham equations with machine learning. Nature Communications, 2017, 8, 872.	12.8	485
47	Leading corrections to local approximations. II. The case with turning points. Physical Review B, 2017, 95, .	3.2	11
48	Direct Extraction of Excitation Energies from Ensemble Density-Functional Theory. Physical Review Letters, 2017, 119, 033003.	7.8	38
49	Pure density functional for strong correlation and the thermodynamic limit from machine learning. Physical Review B, 2016, 94, .	3.2	83
50	Locality of correlation in density functional theory. Journal of Chemical Physics, 2016, 145, 054112.	3.0	35
51	Understanding machine-learned density functionals. International Journal of Quantum Chemistry, 2016, 116, 819-833.	2.0	132
52	Thermal Density Functional Theory: Time-Dependent Linear Response and Approximate Functionals from the Fluctuation-Dissipation Theorem. Physical Review Letters, 2016, 116, 233001.	7.8	53
53	Accurate atomic quantum defects from particle-particle random phase approximation. Molecular Physics, 2016, 114, 1189-1198.	1.7	4
54	Almost exact exchange at almost no computational cost in electronic structure. Physical Review A, 2015, 92, .	2.5	11

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55	One-dimensional mimicking of electronic structure: The case for exponentials. Physical Review B, 2015, 91, .	3.2	28
56	Density functional description of Coulomb blockade: Adiabatic versus dynamic exchange correlation. Physical Review B, 2015, 91, .	3.2	12
57	Understanding kernel ridge regression: Common behaviors from simple functions to density functionals. International Journal of Quantum Chemistry, 2015, 115, 1115-1128.	2.0	89
58	Nonlinear gradient denoising: Finding accurate extrema from inaccurate functional derivatives. International Journal of Quantum Chemistry, 2015, 115, 1102-1114.	2.0	21
59	Corrections to Thomas-Fermi Densities at Turning Points and Beyond. Physical Review Letters, 2015, 114, 050401.	7.8	23
60	Quantum critical benchmark for electronic structure theory. Physical Review A, 2015, 91, .	2.5	5
61	DFT: A Theory Full of Holes?. Annual Review of Physical Chemistry, 2015, 66, 283-304.	10.8	149
62	Improved DFT Potential Energy Surfaces via Improved Densities. Journal of Physical Chemistry Letters, 2015, 6, 3802-3807.	4.6	79
63	Gedanken densities and exact constraints in density functional theory. Journal of Chemical Physics, 2014, 140, 18A533.	3.0	82
64	Exact and approximate Kohn-Sham potentials in ensemble density-functional theory. Physical Review A, 2014, 90, .	2.5	48
65	Ions in solution: Density corrected density functional theory (DC-DFT). Journal of Chemical Physics, 2014, 140, 18A528.	3.0	87
66	Kohn-Sham calculations with the exact functional. Physical Review B, 2014, 90, .	3.2	39
67	Excitations and benchmark ensemble density functional theory for two electrons. Journal of Chemical Physics, 2014, 140, 18A541.	3.0	42
68	Communication: Testing and using the Lewin-Lieb bounds in density functional theory. Journal of Chemical Physics, 2014, 141, 241105.	3.0	10
69	DFT in a nutshell. International Journal of Quantum Chemistry, 2013, 113, 96-101.	2.0	143
70	Guaranteed Convergence of the Kohn-Sham Equations. Physical Review Letters, 2013, 111, 093003.	7.8	39
71	Understanding and Reducing Errors in Density Functional Calculations. Physical Review Letters, 2013, 111, 073003.	7.8	271
72	Potential functionals versus density functionals. Physical Review A, 2013, 88, .	2.5	25

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73	Orbital-free bond breaking via machine learning. Journal of Chemical Physics, 2013, 139, 224104.	3.0	92
74	Kernels, Pre-images and Optimization. , 2013, , 245-259.		10
75	Finding Density Functionals with Machine Learning. Physical Review Letters, 2012, 108, 253002.	7.8	495
76	One-Dimensional Continuum Electronic Structure with the Density-Matrix Renormalization Group and Its Implications for Density-Functional Theory. Physical Review Letters, 2012, 109, 056402.	7.8	73
77	Perspective on density functional theory. Journal of Chemical Physics, 2012, 136, 150901.	3.0	1,236
78	Reference electronic structure calculations in one dimension. Physical Chemistry Chemical Physics, 2012, 14, 8581.	2.8	63
79	Electronic Structure via Potential Functional Approximations. Physical Review Letters, 2011, 106, 236404.	7.8	39
80	Communication: Avoiding unbound anions in density functional calculations. Journal of Chemical Physics, 2011, 134, 171103.	3.0	93
81	Communication: Ionization potentials in the limit of large atomic number. Journal of Chemical Physics, 2010, 133, 241103.	3.0	40
82	Leading corrections to local approximations. Physical Review B, 2010, 81, .	3.2	27
83	Accuracy of Electron Affinities of Atoms in Approximate Density Functional Theory. Journal of Physical Chemistry Letters, 2010, 1, 2124-2129.	4.6	66
84	Finding electron affinities with approximate density functionals. Molecular Physics, 2010, 108, 2687-2701.	1.7	20
85	Condition on the Kohn-Sham kinetic energy and modern parametrization of the Thomas-Fermi density. Journal of Chemical Physics, 2009, 130, 034107.	3.0	63
86	Adiabatic connection for strictly correlated electrons. Journal of Chemical Physics, 2009, 131, 124124.	3.0	21
87	Must Kohn-Sham oscillator strengths be accurate at threshold?. Journal of Chemical Physics, 2009, 131, 114308.	3.0	6
88	Special Issue in Honor of John P. Perdew for His 65th Birthday. Journal of Chemical Theory and Computation, 2009, 5, 675-678.	5.3	4
89	Time-dependent density functional theory of high excitations: to infinity, and beyond. Physical Chemistry Chemical Physics, 2009, 11, 4437.	2.8	30
90	Density Functional Partition Theory with Fractional Occupations. Journal of Chemical Theory and Computation, 2009, 5, 827-833.	5.3	68

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91	Charge Transfer in Partition Theory. Journal of Physical Chemistry A, 2009, 113, 2183-2192.	2.5	13
92	Non-empirical derivation of the parameter in the B88 exchange functional. Canadian Journal of Chemistry, 2009, 87, 1485-1491.	1.1	85
93	Restoring the Density-Gradient Expansion for Exchange in Solids and Surfaces. Physical Review Letters, 2008, 100, 136406.	7.8	8,139
94	Comment on "Critique of the foundations of time-dependent density-functional theory". Physical Review A, 2008, 78, .	2.5	34
95	Semiclassical Origins of Density Functionals. Physical Review Letters, 2008, 100, 256406.	7.8	85
96	Time-Dependent Density Functional Calculation of $\hat{e}^{\frac{i}{\hbar} \int_{-\infty}^{\infty} dt \int d^3r \mathbf{r} \cdot \nabla \times \mathbf{A}(\mathbf{r}, t)}$ Scattering. Physical Review Letters, 2007, 99, 043005.	7.8	21
97	Comment on "Analysis of Floquet formulation of time-dependent density-functional theory". Chem. Phys. Lett. 433 (2006) 204]. Chemical Physics Letters, 2007, 441, 167-169.	2.6	13
98	Partition Theory: A Very Simple Illustration. Journal of Physical Chemistry A, 2007, 111, 12447-12453.	2.5	15
99	Relevance of the Slowly Varying Electron Gas to Atoms, Molecules, and Solids. Physical Review Letters, 2006, 97, 223002.	7.8	94
100	A new challenge for time-dependent density functional theory. Chemical Physics Letters, 2006, 431, 410-414.	2.6	9
101	The quantum defect: The true measure of time-dependent density-functional results for atoms. Journal of Chemical Physics, 2006, 124, 094102.	3.0	15
102	Zero-bias molecular electronics: Exchange-correlation corrections to Landauer's formula. Physical Review B, 2006, 73, .	3.2	164
103	Density Functional Theory of the Electrical Conductivity of Molecular Devices. Physical Review Letters, 2005, 94, 146803.	7.8	121
104	Continuum states from time-dependent density functional theory. Journal of Chemical Physics, 2005, 122, 144103.	3.0	15
105	Rydberg Transition Frequencies from the Local Density Approximation. Physical Review Letters, 2005, 95, 163006.	7.8	31
106	Chapter 2 Time-Dependent Density Functional Theory in Quantum Chemistry. Annual Reports in Computational Chemistry, 2005, , 19-30.	1.7	48
107	Relations between coordinate and potential scaling in the high-density limit. Journal of Chemical Physics, 2005, 122, 134108.	3.0	6
108	Time-dependent density functional theory: Past, present, and future. Journal of Chemical Physics, 2005, 123, 062206.	3.0	791

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109	Self-Interaction Errors in Density-Functional Calculations of Electronic Transport. Physical Review Letters, 2005, 95, 146402.	7.8	292
110	Double excitations within time-dependent density functional theory linear response. Journal of Chemical Physics, 2004, 120, 5932-5937.	3.0	431
111	Adiabatic connection for near degenerate excited states. Physical Review A, 2004, 69, .	2.5	26
112	A dressed TDDFT treatment of the 21Ag states of butadiene and hexatriene. Chemical Physics Letters, 2004, 389, 39-42.	2.6	192
113	Excitation energies from time-dependent density-functional theory beyond the adiabatic approximation. Journal of Chemical Physics, 2004, 121, 28.	3.0	65
114	Accurate Rydberg Excitations from the Local Density Approximation. Physical Review Letters, 2003, 91, 263001.	7.8	41
115	Testing the kinetic energy functional: Kinetic energy density as a density functional. Journal of Chemical Physics, 2003, 118, 8140-8148.	3.0	38
116	TEN TOPICAL QUESTIONS IN TIME-DEPENDENT DENSITY FUNCTIONAL THEORY. , 2002, , 1186-1225.		21
117	Memory in Time-Dependent Density Functional Theory. Physical Review Letters, 2002, 89, 023002.	7.8	159
118	Correlation in time-dependent density-functional theory. Journal of Chemical Physics, 2002, 117, 72-81.	3.0	46
119	Theoretical Investigation of the Ground and Excited States of Coumarin 151 and Coumarin 120. Journal of Physical Chemistry A, 2002, 106, 9294-9305.	2.5	156
120	On the Floquet formulation of time-dependent density functional theory. Chemical Physics Letters, 2002, 359, 237-240.	2.6	25
121	Symmetry and degeneracy in density functional theory. International Journal of Quantum Chemistry, 2001, 85, 432-435.	2.0	7
122	Demonstration of initial-state dependence in time-dependent density-functional theory. Physical Review A, 2001, 63, .	2.5	66
123	Can optimized effective potentials be determined uniquely?. Journal of Chemical Physics, 2001, 115, 1635-1649.	3.0	184
124	Excitation energies from time-dependent density functional theory using exact and approximate potentials. International Journal of Quantum Chemistry, 2000, 80, 534-554.	2.0	57
125	Adiabatic connection from accurate wave-function calculations. Journal of Chemical Physics, 2000, 112, 5292-5297.	3.0	40
126	Total energy density as an interpretative tool. Journal of Chemical Physics, 2000, 113, 2990-2994.	3.0	69

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127	Exact high-density limit of correlation potential for two-electron density. Journal of Chemical Physics, 1999, 110, 10262-10268.	3.0	54
128	Several Theorems in Time-Dependent Density Functional Theory. Physical Review Letters, 1999, 82, 378-381.	7.8	82
129	Virial exchange-correlation energy density in Hooke's atom. International Journal of Quantum Chemistry, 1998, 69, 533-540.	2.0	16
130	Unambiguous exchange-correlation energy density for Hooke's atom. International Journal of Quantum Chemistry, 1998, 70, 583-589.	2.0	15
131	Exchange-Correlation Energy Density from Virial Theorem. Journal of Physical Chemistry A, 1998, 102, 4911-4917.	2.5	86
132	Nonlocality of the density functional for exchange and correlation: Physical origins and chemical consequences. Journal of Chemical Physics, 1998, 108, 1522-1531.	3.0	88
133	Why semilocal functionals work: Accuracy of the on-top pair density and importance of system averaging. Journal of Chemical Physics, 1998, 109, 3760-3771.	3.0	167
134	Unambiguous exchange-correlation energy density. Journal of Chemical Physics, 1998, 109, 8161-8167.	3.0	109
135	Why Density-Gradient Corrections Improve Atomization Energies and Barrier Heights. Advances in Quantum Chemistry, 1998, 33, 1-9.	0.8	2
136	Unambiguous exchange-correlation energy density for Hooke's atom. International Journal of Quantum Chemistry, 1998, 70, 583-589.	2.0	2
137	Distributions and averages of electron density parameters: Explaining the effects of gradient corrections. Journal of Chemical Physics, 1997, 106, 10184-10193.	3.0	144
138	Generalized Gradient Approximation Made Simple [Phys. Rev. Lett. 77, 3865 (1996)]. Physical Review Letters, 1997, 78, 1396-1396.	7.8	12,087
139	On-top pair-density interpretation of spin density functional theory, with applications to magnetism. International Journal of Quantum Chemistry, 1997, 61, 197-205.	2.0	97
140	Why the generalized gradient approximation works and how to go beyond it. International Journal of Quantum Chemistry, 1997, 61, 287-293.	2.0	126
141	Density-gradient analysis for density functional theory: Application to atoms. International Journal of Quantum Chemistry, 1997, 61, 835-845.	2.0	81
142	Coupling-constant dependence of atomization energies. International Journal of Quantum Chemistry, 1997, 64, 285-295.	2.0	174
143	The adiabatic connection method: a non-empirical hybrid. Chemical Physics Letters, 1997, 265, 115-120.	2.6	212
144	Why the generalized gradient approximation works and how to go beyond it. , 1997, 61, 287.		5

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145	Density-gradient analysis for density functional theory: Application to atoms. , 1997, 61, 835.		4
146	Coupling-constant dependence of atomization energies. , 1997, 64, 285.		4
147	Coupling-constant dependence of atomization energies. International Journal of Quantum Chemistry, 1997, 64, 285-295.	2.0	3
148	Local and Gradient-Corrected Density Functionals. ACS Symposium Series, 1996, , 453-462.	0.5	56
149	Generalized gradient approximation for the exchange-correlation hole of a many-electron system. Physical Review B, 1996, 54, 16533-16539.	3.2	5,433
150	Generalized Gradient Approximation Made Simple. Physical Review Letters, 1996, 77, 3865-3868.	7.8	157,044
151	Rationale for mixing exact exchange with density functional approximations. Journal of Chemical Physics, 1996, 105, 9982-9985.	3.0	4,987
152	Comparison shopping for a gradient-corrected density functional. International Journal of Quantum Chemistry, 1996, 57, 309-319.	2.0	276
153	Long-range asymptotic behavior of ground-state wave functions, one-electron matrices, and pair densities. Journal of Chemical Physics, 1996, 105, 2798-2803.	3.0	51
154	Improving energies by using exact electron densities. Physical Review A, 1996, 53, R2915-R2917.	2.5	22
155	Comparison shopping for a gradient-corrected density functional. International Journal of Quantum Chemistry, 1996, 57, 309-319.	2.0	3
156	Real-space analysis of the exchange-correlation energy. International Journal of Quantum Chemistry, 1995, 56, 199-210.	2.0	33
157	Escaping the symmetry dilemma through a pair-density interpretation of spin-density functional theory. Physical Review A, 1995, 51, 4531-4541.	2.5	335
158	DENSITY FUNCTIONALS AND SMALL INTERPARTICLE SEPARATIONS IN ELECTRONIC SYSTEMS. Modern Physics Letters B, 1995, 09, 829-838.	1.9	6
159	Semilocal density functionals for exchange and correlation: Theory and applications. Theoretical and Computational Chemistry, 1995, 2, 29-74.	0.4	13
160	PROBING SURFACE LATTICE DYNAMICS WITH HYPERTHERMAL ION SCATTERING. Surface Review and Letters, 1994, 01, 175-185.	1.1	2
161	Is the Local Density Approximation Exact for Short Wavelength Fluctuations?. Physical Review Letters, 1994, 73, 1283-1286.	7.8	56
162	Validity of the extended electron-electron cusp condition. Physical Review A, 1994, 50, 297-304.	2.5	12

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163	Limitations of the Trajectory Approximation in Atom-Surface Scattering. Physical Review Letters, 1994, 73, 2768-2771.	7.8	16
164	Anomalous charge oscillations in the dynamical response of metals. Physical Review B, 1994, 49, 11397-11404.	3.2	7
165	Vibrational dephasing at surfaces: The role of cubic anharmonicity and Fermi resonances. Physical Review B, 1993, 47, 15869-15889.	3.2	13
166	Nearly elastic scattering and the trajectory approximation. Physical Review B, 1993, 47, 12852-12864.	3.2	22
167	Crystallinity effects on the surface optical response in metals. Physical Review B, 1993, 48, 14599-14607.	3.2	14
168	Angle-resolved electron-energy-loss study of Al/Si(111). Physical Review B, 1993, 48, 12063-12071.	3.2	6
169	Comparison shopping for a gradient-corrected density functional. , 0, .		5
170	On-top pair-density interpretation of spin density functional theory, with applications to magnetism. , 0, .		3
171	Unambiguous exchangeâ€“correlation energy density for Hooke's atom. , 0, .		1
172	Excitation energies from time-dependent density functional theory using exact and approximate potentials. , 0, .		2
173	Speeding Up DFT Calculations with Machine Learning. ChemistryViews, 0, , .	0.0	0