# Kieron Burke

List of Publications by Year
in descending order

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|---|---|---|---|
| 173 papers | 200,163 citations | 18436 62 h-index | 6113 159 g-index |
| 179 all docs | 179 docs citations | 179 times ranked | 99795 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Density-Corrected DFT Explained: Questions and Answers. Journal of Chemical Theory and Computation, 2022, 18, 817-827. | 2.3 | 33 |
| 2 | How Well Does Kohnâ€“Sham Regularizer Work for Weakly Correlated Systems?. Journal of Physical Chemistry Letters, 2022, 13, 2540-2547. | 2.1 | 6 |
| 3 | Improving Results by Improving Densities: Density-Corrected Density Functional Theory. Journal of the American Chemical Society, 2022, 144, 6625-6639. | 6.6 | 45 |
| 4 | Correlation energy of the uniform electron gas determined by ground-state conditional probability density functional theory. Physical Review B, 2022, 105, . | 1.1 | 2 |
| 5 | Machine learning and density functional theory. Nature Reviews Physics, 2022, 4, 357-358. | 11.9 | 37 |
| 6 | Conditional probability density functional theory. Physical Review B, 2022, 105, . | 1.1 | 4 |
| 7 | Uncommonly accurate energies for the general quartic oscillator. International Journal of Quantum Chemistry, 2021, 121, e26554. | 1.0 | 10 |
| 8 | Density Sensitivity of Empirical Functionals. Journal of Physical Chemistry Letters, 2021, 12, 800-807. | 2.1 | 29 |
| 9 | Calculation and interpretation of classical turning surfaces in solids. Npj Computational Materials, 2021, 7, . | 3.5 | 6 |
| 10 | Learning to Approximate Density Functionals. Accounts of Chemical Research, 2021, 54, 818-826. | 7.6 | 50 |
| 11 | Explaining and Fixing DFT Failures for Torsional Barriers. Journal of Physical Chemistry Letters, 2021, 12, 2796-2804. | 2.1 | 23 |
| 12 | Bob Cave Memorial. Journal of Physical Chemistry A, 2021, 125, 4037-4038. | 1.1 | 0 |
| 13 | Response to comment. International Journal of Quantum Chemistry, 2021, 121, e26767. | 1.0 | 0 |
| 14 | Kohn-Sham Equations as Regularizer: Building Prior Knowledge into Machine-Learned Physics. Physical Review Letters, 2021, 126, 036401. | 2.9 | 89 |
| 15 | Exact and approximate energy sums in potential wells. Journal of Physics A: Mathematical and Theoretical, 2020, 53, 095203. | 0.7 | 9 |
| 16 | Quantum chemical accuracy from density functional approximations via machine learning. Nature Communications, 2020, 11, 5223. | 5.8 | 187 |
| 17 | Retrospective on a decade of machine learning for chemical discovery. Nature Communications, 2020, 11, 4895. | 5.8 | 96 |
| 18 | Measuring Density-Driven Errors Using Kohnâ€“Sham Inversion. Journal of Chemical Theory and Computation, 2020, 16, 5014-5023. | 2.3 | 28 |

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| 19 | Challenges for large scale simulation: general discussion. Faraday Discussions, 2020, 224, 309-332. | 1.6 | 2 |
| 20 | New density-functional approximations and beyond: general discussion. Faraday Discussions, 2020, 224, 166-200. | 1.6 | 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. | 2.3 | 5 |
| 22 | New approaches to study excited states in density functional theory: general discussion. Faraday Discussions, 2020, 224, 483-508. | 1.6 | 2 |
| 23 | Quantifying and Understanding Errors in Molecular Geometries. Journal of Physical Chemistry Letters, 2020, 11, 9957-9964. | 2.1 | 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. | 1.2 | 10 |
| 25 | Deriving approximate functionals with asymptotics. Faraday Discussions, 2020, 224, 98-125. | 1.6 | 3 |
| 26 | MAP: An MP2 Accuracy Predictor for Weak Interactions from Adiabatic Connection Theory. Journal of Chemical Theory and Computation, 2020, 16, 4141-4149. | 2.3 | 10 |
| 27 | Leading correction to the local density approximation of the kinetic energy in one dimension. Journal of Chemical Physics, 2020, 152, 081102. | 1.2 | 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. | 2.9 | 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. | 0.3 | 6 |
| 31 | Density Functional Analysis: The Theory of Density-Corrected DFT. Journal of Chemical Theory and Computation, 2019, 15, 6636-6646. | 2.3 | 66 |
| 32 | Halogen and Chalcogen Binding Dominated by Density-Driven Errors. Journal of Physical Chemistry Letters, 2019, 10, 295-301. | 2.1 | 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. | 2.3 | 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, . | 1.1 | 4 |
| 36 | Accurate double excitations from ensemble density functional calculations. Journal of Chemical Physics, 2018, 149, 134103. | 1.2 | 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. | 2.1 | 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. | 1.2 | 33 |
| 40 | Guest Editorial: Special Topic on Data-Enabled Theoretical Chemistry. Journal of Chemical Physics, 2018, 148, 241401. | 1.2 | 77 |
| 41 | Linear response time-dependent density functional theory of the Hubbard dimer. European Physical Journal B, 2018, 91, 1. | 0.6 | 33 |
| 42 | Can exact conditions improve machine-learned density functionals?. Journal of Chemical Physics, 2018, 148, 241743. | 1.2 | 39 |
| 43 | Deriving uniform semiclassical approximations for one-dimensional fermionic systems. Journal of Chemical Physics, 2018, 148, 194103. | 1.2 | 10 |
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| 46 | Bypassing the Kohn-Sham equations with machine learning. Nature Communications, 2017, 8, 872. | 5.8 | 485 |
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| 48 | Direct Extraction of Excitation Energies from Ensemble Density-Functional Theory. Physical Review Letters, 2017, 119, 033003. | 2.9 | 38 |
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| 50 | Locality of correlation in density functional theory. Journal of Chemical Physics, 2016, 145, 054112. | 1.2 | 35 |
| 51 | Understanding machineâ€learned density functionals. International Journal of Quantum Chemistry, 2016, 116, 819-833. | 1.0 | 132 |
| 52 | Thermal Density Functional Theory: Time-Dependent Linear Response and Approximate Functionals from the Fluctuation-Dissipation Theorem. Physical Review Letters, 2016, 116, 233001. | 2.9 | 53 |
| 53 | Accurate atomic quantum defects from particleâ€“particle random phase approximation. Molecular Physics, 2016, 114, 1189-1198. | 0.8 | 4 |
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| 56 | Density functional description of Coulomb blockade: Adiabatic versus dynamic exchange correlation. Physical Review B, 2015, 91, . | 1.1 | 12 |
| 57 | Understanding kernel ridge regression: Common behaviors from simple functions to density functionals. International Journal of Quantum Chemistry, 2015, 115, 1115-1128. | 1.0 | 89 |
| 58 | Nonlinear gradient denoising: Finding accurate extrema from inaccurate functional derivatives. International Journal of Quantum Chemistry, 2015, 115, 1102-1114. | 1.0 | 21 |
| 59 | Corrections to Thomas-Fermi Densities at Turning Points and Beyond. Physical Review Letters, 2015, 114, 050401. | 2.9 | 23 |
| 60 | Quantum critical benchmark for electronic structure theory. Physical Review A, 2015, 91, . | 1.0 | 5 |
| 61 | DFT: A Theory Full of Holes?. Annual Review of Physical Chemistry, 2015, 66, 283-304. | 4.8 | 149 |
| 62 | Improved DFT Potential Energy Surfaces via Improved Densities. Journal of Physical Chemistry Letters, 2015, 6, 3802-3807. | 2.1 | 79 |
| 63 | Gedanken densities and exact constraints in density functional theory. Journal of Chemical Physics, 2014, 140, 18A533. | 1.2 | 82 |
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| 141 | Density-gradient analysis for density functional theory: Application to atoms. International Journal of Quantum Chemistry, 1997, 61, 835-845. | 1.0 | 81 |
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