Kieron Burke

List of Publications by Year
in descending order

173 papers	200,163 citations	18482 62 h-index	5829 161 g-index
179 all docs	179 docs citations	179 times ranked	99795 citing authors

#	Article	IF	Citations
1	Generalized Gradient Approximation Made Simple. Physical Review Letters, 1996, 77, 3865-3868.	7.8	157,044
2	Generalized Gradient Approximation Made Simple [Phys. Rev. Lett. 77, 3865 (1996)]. Physical Review Letters, 1997, 78, 1396-1396.	7.8	12,087
3	Restoring the Density-Gradient Expansion for Exchange in Solids and Surfaces. Physical Review Letters, 2008, 100, 136406.	7.8	8,139
4	Generalized gradient approximation for the exchange-correlation hole of a many-electron system. Physical Review B, 1996, 54, 16533-16539.	3.2	5,433
5	Rationale for mixing exact exchange with density functional approximations. Journal of Chemical Physics, 1996, 105, 9982-9985.	3.0	4,987
6	Perspective on density functional theory. Journal of Chemical Physics, 2012, 136, 150901.	3.0	1,236
7	Time-dependent density functional theory: Past, present, and future. Journal of Chemical Physics, 2005, 123, 062206.	3.0	791
8	Finding Density Functionals with Machine Learning. Physical Review Letters, 2012, 108, 253002.	7.8	495
9	Bypassing the Kohn-Sham equations with machine learning. Nature Communications, 2017, 8, 872.	12.8	485
10	Double excitations within time-dependent density functional theory linear response. Journal of Chemical Physics, 2004, 120, 5932-5937.	3.0	431
11	Understanding band gaps of solids in generalized Kohnâ€“Sham theory. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2801-2806.	7.1	423
12	Escaping the symmetry dilemma through a pair-density interpretation of spin-density functional theory. Physical Review A, 1995, 51, 4531-4541.	2.5	335
13	Self-Interaction Errors in Density-Functional Calculations of Electronic Transport. Physical Review Letters, 2005, 95, 146402.	7.8	292
14	Comparison shopping for a gradient-corrected density functional. International Journal of Quantum Chemistry, 1996, 57, 309-319.	2.0	276
15	Understanding and Reducing Errors in Density Functional Calculations. Physical Review Letters, 2013, 111, 073003.	7.8	271
16	The adiabatic connection method: a non-empirical hybrid. Chemical Physics Letters, 1997, 265, 115-120.	2.6	212
17	A dressed TDDFT treatment of the 21Ag states of butadiene and hexatriene. Chemical Physics Letters, 2004, 389, 39-42.	2.6	192
18	Quantum chemical accuracy from density functional approximations via machine learning. Nature Communications, 2020, 11, 5223.	12.8	187

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19	Can optimized effective potentials be determined uniquely?. Journal of Chemical Physics, 2001, 115, 1635-1649.	3.0	184
20	Coupling-constant dependence of atomization energies. International Journal of Quantum Chemistry, 1997, 64, 285-295.	2.0	174
21	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
22	Zero-bias molecular electronics: Exchange-correlation corrections to Landauer's formula. Physical Review B, 2006, 73, .	3.2	164
23	Memory in Time-Dependent Density Functional Theory. Physical Review Letters, 2002, 89, 023002.	7.8	159
24	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
25	DFT: A Theory Full of Holes?. Annual Review of Physical Chemistry, 2015, 66, 283-304.	10.8	149
26	Distributions and averages of electron density parameters: Explaining the effects of gradient corrections. Journal of Chemical Physics, 1997, 106, 10184-10193.	3.0	144
27	DFT in a nutshell. International Journal of Quantum Chemistry, 2013, 113, 96-101.	2.0	143
28	Understanding machineâ€learned density functionals. International Journal of Quantum Chemistry, 2016, 116, 819-833.	2.0	132
29	Why the generalized gradient approximation works and how to go beyond it. International Journal of Quantum Chemistry, 1997, 61, 287-293.	2.0	126
30	Density Functional Theory of the Electrical Conductivity of Molecular Devices. Physical Review Letters, 2005, 94, 146803.	7.8	121
31	Unambiguous exchange-correlation energy density. Journal of Chemical Physics, 1998, 109, 8161-8167.	3.0	109
32	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
33	Retrospective on a decade of machine learning for chemical discovery. Nature Communications, 2020, 11, 4895.	12.8	96
34	Relevance of the Slowly Varying Electron Gas to Atoms, Molecules, and Solids. Physical Review Letters, 2006, 97, 223002.	7.8	94
35	Communication: Avoiding unbound anions in density functional calculations. Journal of Chemical Physics, 2011, 134, 171103.	3.0	93
36	The Importance of Being Inconsistent. Annual Review of Physical Chemistry, 2017, 68, 555-581.	10.8	93

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37	Orbital-free bond breaking via machine learning. Journal of Chemical Physics, 2013, 139, 224104.	3.0	92
38	Understanding kernel ridge regression: Common behaviors from simple functions to density functionals. International Journal of Quantum Chemistry, 2015, 115, 1115-1128.	2.0	89
39	Kohn-Sham Equations as Regularizer: Building Prior Knowledge into Machine-Learned Physics. Physical Review Letters, 2021, 126, 036401.	7.8	89
40	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
41	Ions in solution: Density corrected density functional theory (DC-DFT). Journal of Chemical Physics, 2014, 140, 18A528.	3.0	87
42	Exchangeâ^'Correlation Energy Density from Virial Theorem. Journal of Physical Chemistry A, 1998, 102, 4911-4917.	2.5	86
43	Semiclassical Origins of Density Functionals. Physical Review Letters, 2008, 100, 256406.	7.8	85
44	Non-empirical derivation of the parameter in the B88 exchange functional. Canadian Journal of Chemistry, 2009, 87, 1485-1491.	1.1	85
45	Pure density functional for strong correlation and the thermodynamic limit from machine learning. Physical Review B, 2016, 94, .	3.2	83
46	Several Theorems in Time-Dependent Density Functional Theory. Physical Review Letters, 1999, 82, 378-381.	7.8	82
47	Gedanken densities and exact constraints in density functional theory. Journal of Chemical Physics, 2014, 140, 18A533.	3.0	82
48	Density-gradient analysis for density functional theory: Application to atoms. International Journal of Quantum Chemistry, 1997, 61, 835-845.	2.0	81
49	Improved DFT Potential Energy Surfaces via Improved Densities. Journal of Physical Chemistry Letters, 2015, 6, 3802-3807.	4.6	79
50	Guest Editorial: Special Topic on Data-Enabled Theoretical Chemistry. Journal of Chemical Physics, 2018, 148, 241401.	3.0	77
51	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
52	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
53	Total energy density as an interpretative tool. Journal of Chemical Physics, 2000, 113, 2990-2994.	3.0	69
54	Density Functional Partition Theory with Fractional Occupations. Journal of Chemical Theory and Computation, 2009, 5, 827-833.	5.3	68

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55	Quantifying Density Errors in DFT. Journal of Physical Chemistry Letters, 2018, 9, 6385-6392.	4.6	67
56	Demonstration of initial-state dependence in time-dependent density-functional theory. Physical Review A, 2001, 63, .	2.5	66
57	Accuracy of Electron Affinities of Atoms in Approximate Density Functional Theory. Journal of Physical Chemistry Letters, 2010, 1, 2124-2129.	4.6	66
58	Density Functional Analysis: The Theory of Density-Corrected DFT. Journal of Chemical Theory and Computation, 2019, 15, 6636-6646.	5.3	66
59	Excitation energies from time-dependent density-functional theory beyond the adiabatic approximation. Journal of Chemical Physics, 2004, 121, 28.	3.0	65
60	Condition on the Kohnâ€“Sham kinetic energy and modern parametrization of the Thomasâ€“Fermi density. Journal of Chemical Physics, 2009, 130, 034107.	3.0	63
61	Reference electronic structure calculations in one dimension. Physical Chemistry Chemical Physics, 2012, 14, 8581.	2.8	63
62	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
63	Is the Local Density Approximation Exact for Short Wavelength Fluctuations?. Physical Review Letters, 1994, 73, 1283-1286.	7.8	56
64	Local and Gradient-Corrected Density Functionals. ACS Symposium Series, 1996, , 453-462.	0.5	56
65	Exact high-density limit of correlation potential for two-electron density. Journal of Chemical Physics, 1999, 110, 10262-10268.	3.0	54
66	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
67	Longâ€range asymptotic behavior of groundâ€state wave functions, oneâ€matrices, and pair densities. Journal of Chemical Physics, 1996, 105, 2798-2803.	3.0	51
68	Learning to Approximate Density Functionals. Accounts of Chemical Research, 2021, 54, 818-826.	15.6	50
69	Chapter 2 Time-Dependent Density Functional Theoryin Quantum Chemistry. Annual Reports in Computational Chemistry, 2005, , 19-30.	1.7	48
70	Exact and approximate Kohn-Sham potentials in ensemble density-functional theory. Physical Review A, 2014, 90, .	2.5	48
71	Correlation in time-dependent density-functional theory. Journal of Chemical Physics, 2002, 117, 72-81.	3.0	46
72	Improving Results by Improving Densities: Density-Corrected Density Functional Theory. Journal of the American Chemical Society, 2022, 144, 6625-6639.	13.7	45

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73	Halogen and Chalcogen Binding Dominated by Density-Driven Errors. Journal of Physical Chemistry Letters, 2019, 10, 295-301.	4.6	43
74	Excitations and benchmark ensemble density functional theory for two electrons. Journal of Chemical Physics, 2014, 140, 18A541.	3.0	42
75	Accurate Rydberg Excitations from the Local Density Approximation. Physical Review Letters, 2003, 91, 263001.	7.8	41
76	Adiabatic connection from accurate wave-function calculations. Journal of Chemical Physics, 2000, 112, 5292-5297.	3.0	40
77	Communication: Ionization potentials in the limit of large atomic number. Journal of Chemical Physics, 2010, 133, 241103.	3.0	40
78	Electronic Structure via Potential Functional Approximations. Physical Review Letters, 2011, 106, 236404.	7.8	39
79	Guaranteed Convergence of the Kohn-Sham Equations. Physical Review Letters, 2013, 111, 093003.	7.8	39
80	Kohn-Sham calculations with the exact functional. Physical Review B, 2014, 90, .	3.2	39
81	Can exact conditions improve machine-learned density functionals?. Journal of Chemical Physics, 2018, 148, 241743.	3.0	39
82	Testing the kinetic energy functional: Kinetic energy density as a density functional. Journal of Chemical Physics, 2003, 118, 8140-8148.	3.0	38
83	Direct Extraction of Excitation Energies from Ensemble Density-Functional Theory. Physical Review Letters, 2017, 119, 033003.	7.8	38
84	Quantifying and Understanding Errors in Molecular Geometries. Journal of Physical Chemistry Letters, 2020, 11, 9957-9964.	4.6	37
85	Machine learning and density functional theory. Nature Reviews Physics, 2022, 4, 357-358.	26.6	37
86	Locality of correlation in density functional theory. Journal of Chemical Physics, 2016, 145, 054112.	3.0	35
87	Comment on â€œCritique of the foundations of time-dependent density-functional theoryâ€. Physical Review A, 2008, 78, .	2.5	34
88	Real-space analysis of the exchange-correlation energy. International Journal of Quantum Chemistry, 1995, 56, 199-210.	2.0	33
89	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
90	Linear response time-dependent density functional theory of the Hubbard dimer. European Physical Journal B, 2018, 91, 1.	1.5	33

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91	Density-Corrected DFT Explained: Questions and Answers. Journal of Chemical Theory and Computation, 2022, 18, 817-827.	5.3	33
92	Rydberg Transition Frequencies from the Local Density Approximation. Physical Review Letters, 2005, 95, 163006.	7.8	31
93	Time-dependent density functional theory of high excitations: to infinity, and beyond. Physical Chemistry Chemical Physics, 2009, 11, 4437.	2.8	30
94	Density Sensitivity of Empirical Functionals. Journal of Physical Chemistry Letters, 2021, 12, 800-807.	4.6	29
95	One-dimensional mimicking of electronic structure: The case for exponentials. Physical Review B, 2015, 91, .	3.2	28
96	Measuring Density-Driven Errors Using Kohnâ€“Sham Inversion. Journal of Chemical Theory and Computation, 2020, 16, 5014-5023.	5.3	28
97	Leading corrections to local approximations. Physical Review B, 2010, 81, .	3.2	27
98	Adiabatic connection for near degenerate excited states. Physical Review A, 2004, 69, .	2.5	26
99	Accurate double excitations from ensemble density functional calculations. Journal of Chemical Physics, 2018, 149, 134103.	3.0	26
100	On the Floquet formulation of time-dependent density functional theory. Chemical Physics Letters, 2002, 359, 237-240.	2.6	25
101	Potential functionals versus density functionals. Physical Review A, 2013, 88, .	2.5	25
102	Corrections to Thomas-Fermi Densities at Turning Points and Beyond. Physical Review Letters, 2015, 114, 050401.	7.8	23
103	Explaining and Fixing DFT Failures for Torsional Barriers. Journal of Physical Chemistry Letters, 2021, 12, 2796-2804.	4.6	23
104	Nearly elastic scattering and the trajectory approximation. Physical Review B, 1993, 47, 12852-12864.	3.2	22
105	Improving energies by using exact electron densities. Physical Review A, 1996, 53, R2915-R2917.	2.5	22
106	TEN TOPICAL QUESTIONS IN TIME-DEPENDENT DENSITY FUNCTIONAL THEORY. , 2002, , 1186-1225.		21
107	Time-Dependent Density Functional Calculation of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>e</mml:mi><mml:mtext mathvariant="normal">â^'</mml:mtext><mml:mi mathvariant="normal">H</mml:mi></mml:math>Scattering. Physical Review Letters, 2007, 99, 043005.	7.8	21
108	Adiabatic connection for strictly correlated electrons. Journal of Chemical Physics, 2009, 131, 124124.	3.0	21

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109	Nonlinear gradient denoising: Finding accurate extrema from inaccurate functional derivatives. International Journal of Quantum Chemistry, 2015, 115, 1102-1114.	2.0	21
110	Finding electron affinities with approximate density functionals. Molecular Physics, 2010, 108, 2687-2701.	1.7	20
111	Limitations of the Trajectory Approximation in Atom-Surface Scattering. Physical Review Letters, 1994, 73, 2768-2771.	7.8	16
112	Virial exchange-correlation energy density in Hooke's atom. International Journal of Quantum Chemistry, 1998, 69, 533-540.	2.0	16
113	Unambiguous exchange-correlation energy density for Hooke's atom. International Journal of Quantum Chemistry, 1998, 70, 583-589.	2.0	15
114	Continuum states from time-dependent density functional theory. Journal of Chemical Physics, 2005, 122, 144103.	3.0	15
115	The quantum defect: The true measure of time-dependent density-functional results for atoms. Journal of Chemical Physics, 2006, 124, 094102.	3.0	15
116	Partition Theory:â€‰ A Very Simple Illustration. Journal of Physical Chemistry A, 2007, 111, 12447-12453.	2.5	15
117	Warming Up Density Functional Theory. , 2018, , 249-271.		15
118	Crystallinity effects on the surface optical response in metals. Physical Review B, 1993, 48, 14599-14607.	3.2	14
119	Vibrational dephasing at surfaces: The role of cubic anharmonicity and Fermi resonances. Physical Review B, 1993, 47, 15869-15889.	3.2	13
120	Semilocal density functionals for exchange and correlation: Theory and applications. Theoretical and Computational Chemistry, 1995, 2, 29-74.	0.4	13
121	Comment on â€œAnalysis of Floquet formulation of time-dependent density-functional theoryâ€[Chem. Phys. Lett. 433 (2006) 204]. Chemical Physics Letters, 2007, 441, 167-169.	2.6	13
122	Charge Transfer in Partition Theory. Journal of Physical Chemistry A, 2009, 113, 2183-2192.	2.5	13
123	Validity of the extended electron-electron cusp condition. Physical Review A, 1994, 50, 297-304.	2.5	12
124	Density functional description of Coulomb blockade: Adiabatic versus dynamic exchange correlation. Physical Review B, 2015, 91, .	3.2	12
125	Almost exact exchange at almost no computational cost in electronic structure. Physical Review A, 2015, 92, .	2.5	11
126	Leading corrections to local approximations. II. The case with turning points. Physical Review B, 2017, 95, .	3.2	11

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127	Communication: Testing and using the Lewin-Lieb bounds in density functional theory. Journal of Chemical Physics, 2014, 141, 241105.	3.0	10
128	Deriving uniform semiclassical approximations for one-dimensional fermionic systems. Journal of Chemical Physics, 2018, 148, 194103.	3.0	10
129	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
130	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
131	Uncommonly accurate energies for the general quartic oscillator. International Journal of Quantum Chemistry, 2021, 121, e26554.	2.0	10
132	Kernels, Pre-images and Optimization. , 2013, , 245-259.		10
133	A new challenge for time-dependent density functional theory. Chemical Physics Letters, 2006, 431, 410-414.	2.6	9
134	Exact and approximate energy sums in potential wells. Journal of Physics A: Mathematical and Theoretical, 2020, 53, 095203.	2.1	9
135	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
136	Anomalous charge oscillations in the dynamical response of metals. Physical Review B, 1994, 49, 11397-11404.	3.2	7
137	Symmetry and degeneracy in density functional theory. International Journal of Quantum Chemistry, 2001, 85, 432-435.	2.0	7
138	Angle-resolved electron-energy-loss study of Al/Si(111). Physical Review B, 1993, 48, 12063-12071.	3.2	6
139	DENSITY FUNCTIONALS AND SMALL INTERPARTICLE SEPARATIONS IN ELECTRONIC SYSTEMS. Modern Physics Letters B, 1995, 09, 829-838.	1.9	6
140	Relations between coordinate and potential scaling in the high-density limit. Journal of Chemical Physics, 2005, 122, 134108.	3.0	6
141	Must Kohnâ€“Sham oscillator strengths be accurate at threshold?. Journal of Chemical Physics, 2009, 131, 114308.	3.0	6
142	Semiclassical quantization of truncated potentials. European Journal of Physics, 2019, 40, 065403.	0.6	6
143	Leading correction to the local density approximation of the kinetic energy in one dimension. Journal of Chemical Physics, 2020, 152, 081102.	3.0	6
144	Calculation and interpretation of classical turning surfaces in solids. Npj Computational Materials, 2021, 7, .	8.7	6

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145	How Well Does Kohnâ€“Sham Regularizer Work for Weakly Correlated Systems?. Journal of Physical Chemistry Letters, 2022, 13, 2540-2547.	4.6	6
146	Quantum critical benchmark for electronic structure theory. Physical Review A, 2015, 91, .	2.5	5
147	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
148	Comparison shopping for a gradient-corrected density functional. , 0, .		5
149	Why the generalized gradient approximation works and how to go beyond it. , 1997, 61, 287.		5
150	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
151	Accurate atomic quantum defects from particleâ€“particle random phase approximation. Molecular Physics, 2016, 114, 1189-1198.	1.7	4
152	Thermal stitching: Combining the advantages of different quantum fermion solvers. Physical Review B, 2018, 98, .	3.2	4
153	Density-gradient analysis for density functional theory: Application to atoms. , 1997, 61, 835.		4
154	Coupling-constant dependence of atomization energies. , 1997, 64, 285.		4
155	Conditional probability density functional theory. Physical Review B, 2022, 105, .	3.2	4
156	Deriving approximate functionals with asymptotics. Faraday Discussions, 2020, 224, 98-125.	3.2	3
157	Comparison shopping for a gradientâ€corrected density functional. International Journal of Quantum Chemistry, 1996, 57, 309-319.	2.0	3
158	On-top pair-density interpretation of spin density functional theory, with applications to magnetism. , 0, .		3
159	Couplingâ€constant dependence of atomization energies. International Journal of Quantum Chemistry, 1997, 64, 285-295.	2.0	3
160	Recent Developments in Density Functional Approximations. , 2020, , 213-226.		3
161	PROBING SURFACE LATTICE DYNAMICS WITH HYPERTHERMAL ION SCATTERING. Surface Review and Letters, 1994, 01, 175-185.	1.1	2
162	Why Density-Gradient Corrections Improve Atomization Energies and Barrier Heights. Advances in Quantum Chemistry, 1998, 33, 1-9.	0.8	2

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163	Recent Developments in Density Functional Approximations. , 2018, , 1-14.		2
164	Challenges for large scale simulation: general discussion. Faraday Discussions, 2020, 224, 309-332.	3.2	2
165	New approaches to study excited states in density functional theory: general discussion. Faraday Discussions, 2020, 224, 483-508.	3.2	2
166	Unambiguous exchangeâ€“correlation energy density for Hooke's atom. International Journal of Quantum Chemistry, 1998, 70, 583-589.	2.0	2
167	Excitation energies from time-dependent density functional theory using exact and approximate potentials. , 0, .		2
168	Correlation energy of the uniform electron gas determined by ground-state conditional probability density functional theory. Physical Review B, 2022, 105, .	3.2	2
169	New density-functional approximations and beyond: general discussion. Faraday Discussions, 2020, 224, 166-200.	3.2	1
170	Unambiguous exchangeâ€“correlation energy density for Hooke's atom. , 0, .		1
171	Bob Cave Memorial. Journal of Physical Chemistry A, 2021, 125, 4037-4038.	2.5	0
172	Response to comment. International Journal of Quantum Chemistry, 2021, 121, e26767.	2.0	0
173	Speeding Up DFT Calculations with Machine Learning. ChemistryViews, 0, , .	0.0	0