Timothy Gould

List of Publications by Year
in descending order

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74 papers	2,545 citations	218592 26 h-index	197736 49 g-index
142 all docs	142 docs citations	142 times ranked	3056 citing authors

#	Article	IF	Citations
1	Adiabatic Connection for Rangeâ€Separated Hybrid Functionals. Advanced Theory and Simulations, 2022, 5, .	1.3	1
2	Poisoning density functional theory with benchmark sets of difficult systems. Physical Chemistry Chemical Physics, 2022, 24, 6398-6403.	1.3	12
3	Single Excitation Energies Obtained from the Ensemble â€œHOMOâ€“LUMO Gapâ€ Exact Results and Approximations. Journal of Physical Chemistry Letters, 2022, 13, 2452-2458.	2.1	14
4	Band-Structure Engineering of Copper Benzenehexathiol for Reversible Mechanochromism: A First-Principles Study. Journal of Physical Chemistry C, 2022, 126, 11642-11651.	1.5	0
5	Effect of pseudopotential choice on the calculated electron and phonon band structures of palladium hydride and its vacancy defect phases. International Journal of Hydrogen Energy, 2021, 46, 943-954.	3.8	2
6	Ensemble generalized Kohnâ€“Sham theory: The good, the bad, and the ugly. Journal of Chemical Physics, 2021, 154, 094125.	1.2	12
7	Self-Interaction-Corrected Random Phase Approximation. Journal of Chemical Theory and Computation, 2021, 17, 2107-2115.	2.3	2
8	First-principles study of the atomic volume of hydrogen in palladium. Journal of Alloys and Compounds, 2021, 864, 158713.	2.8	4
9	Double excitations in molecules from ensemble density functionals: Theory and approximations. Physical Review A, 2021, 104, .	1.0	10
10	Establishing the accuracy of density functional approaches for the description of noncovalent interactions in ionic liquids. Physical Chemistry Chemical Physics, 2021, 23, 25558-25564.	1.3	5
11	uMBD: A Materials-Ready Dispersion Correction That Uniformly Treats Metallic, Ionic, and van der Waals Bonding. Journal of the American Chemical Society, 2020, 142, 2346-2354.	6.6	29
12	Approximately Self-Consistent Ensemble Density Functional Theory: Toward Inclusion of All Correlations. Journal of Physical Chemistry Letters, 2020, 11, 9907-9912.	2.1	10
13	Establishing the accuracy of density functional approaches for the description of noncovalent interactions in biomolecules. Physical Chemistry Chemical Physics, 2020, 22, 21685-21695.	1.3	4
14	Ensemble Density Functional Theory: Insight from the Fluctuation-Dissipation Theorem. Physical Review Letters, 2020, 125, 233001.	2.9	17
15	Exact Generalized Kohn-Sham Theory for Hybrid Functionals. Physical Review X, 2020, 10, .	2.8	19
16	Hierarchical Co₃O₄@N-Doped Carbon Composite as an Advanced Anode Material for Ultrastable Potassium Storage. ACS Nano, 2020, 14, 5027-5035.	7.3	121
17	Carbon dots derived from human hair for ppb level chloroform sensing in water. Sustainable Materials and Technologies, 2020, 25, e00159.	1.7	21
18	What do we learn from the classical turning surface of the Kohnâ€“Sham potential as electron number is varied continuously?. Journal of Chemical Physics, 2020, 152, 054105.	1.2	1

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19	Density-Driven Correlations in Ensemble Density Functional Theory: Insights from Simple Excitations in Atoms. Australian Journal of Chemistry, 2020, 73, 714.	0.5	12
20	Electrochromic properties of Li4Ti5O12: From visible to infrared spectrum. Applied Physics Letters, 2019, 115, .	1.5	30
21	Density-Driven Correlations in Many-Electron Ensembles: Theory and Application for Excited States. Physical Review Letters, 2019, 123, 016401.	2.9	28
22	Range-separation and the multiple radii functional approximation inspired by the strongly interacting limit of density functional theory. Journal of Chemical Physics, 2019, 151, 184101.	1.2	8
23	Asymptotic behavior of the Hartree-exchange and correlation potentials in ensemble density functional theory. Physical Chemistry Chemical Physics, 2019, 21, 19805-19815.	1.3	14
24	Simple self-interaction correction to random-phase-approximation-like correlation energies. Physical Review A, 2019, 100, .	1.0	13
25	Strong Correlation and Charge Localization in Kohnâ€“Sham Theories with Fractional Orbital Occupations. Journal of Chemical Theory and Computation, 2019, 15, 4907-4914.	2.3	10
26	Polymorphism of bulk boron nitride. Science Advances, 2019, 5, eaau5832.	4.7	33
27	Bridging molecular dynamics and correlated wave-function methods for accurate finite-temperature properties. Physical Review Materials, 2019, 3, .	0.9	16
28	Methods for converging correlation energies within the dielectric matrix formalism. Physical Review B, 2018, 97, .	1.1	2
29	Benchmarking several van der Waals dispersion approaches for the description of intermolecular interactions. Journal of Chemical Physics, 2018, 148, 064112.	1.2	37
30	Charge transfer excitations from exact and approximate ensemble Kohn-Sham theory. Journal of Chemical Physics, 2018, 148, 174101.	1.2	29
31	â€˜Diet GMTKN55â€™ offers accelerated benchmarking through a representative subset approach. Physical Chemistry Chemical Physics, 2018, 20, 27735-27739.	1.3	26
32	Does the exchangeâ€“correlation kernel fxc have a very long-ranged dependence on the groundstate electron density?. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	1
33	Are dispersion corrections accurate outside equilibrium? A case study on benzene. Beilstein Journal of Organic Chemistry, 2018, 14, 1181-1191.	1.3	15
34	Faraday cage screening reveals intrinsic aspects of the van der Waals attraction. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E10295-E10302.	3.3	12
35	Quantum heat engine operating between thermal and spin reservoirs. Physical Review A, 2018, 97, .	1.0	17
36	Evaluation of van der Waals density functionals for layered materials. Physical Review Materials, 2018, 2, .	0.9	71

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37	What Makes a Density Functional Approximation Good? Insights from the Left Fukui Function. Journal of Chemical Theory and Computation, 2017, 13, 2373-2377.	2.3	33
38	Hartree and Exchange in Ensemble Density Functional Theory: Avoiding the Nonuniqueness Disaster. Physical Review Letters, 2017, 119, 243001.	2.9	42
39	MoirÃ©-pattern interlayer potentials in van der Waals materials in the random-phase approximation. Physical Review B, 2017, 96, .	1.1	19
40	Casimirâ€“Polder Size Consistency: A Constraint Violated by Some Dispersion Theories. Journal of Chemical Theory and Computation, 2017, 13, 5829-5833.	2.3	8
41	Surface Adsorption. , 2017, , 387-416.		4
42	How polarizabilities and C6 coefficients actually vary with atomic volume. Journal of Chemical Physics, 2016, 145, 084308.	1.2	13
43	Locality of correlation in density functional theory. Journal of Chemical Physics, 2016, 145, 054112.	1.2	35
44	2D Structures Beyond Graphene. Semiconductors and Semimetals, 2016, 95, 1-33.	0.4	8
45	Layer response theory: Energetics of layered materials from semianalytic high-level theory. Physical Review B, 2016, 93, .	1.1	11
46	A Fractionally Ionic Approach to Polarizability and van der Waals Many-Body Dispersion Calculations. Journal of Chemical Theory and Computation, 2016, 12, 5920-5930.	2.3	90
47	C₆ Coefficients and Dipole Polarizabilities for All Atoms and Many Ions in Rows 1â€“6 of the Periodic Table. Journal of Chemical Theory and Computation, 2016, 12, 3603-3613.	2.3	76
48	An improved model for metal-hydrogen storage tanks â€“ Part 1: Model development. International Journal of Hydrogen Energy, 2016, 41, 3537-3550.	3.8	27
49	An improved model for metal-hydrogen storage tanks â€“ Part 2: Model results. International Journal of Hydrogen Energy, 2016, 41, 3919-3927.	3.8	17
50	Many-body dispersion corrections for periodic systems: an efficient reciprocal space implementation. Journal of Physics Condensed Matter, 2016, 28, 045201.	0.7	86
51	Kohn-Sham potentials in exact density-functional theory at noninteger electron numbers. Physical Review A, 2014, 90, .	1.0	42
52	Density functional theory analysis of structural and electronic properties of orthorhombic perovskite CH₃NH₃PbI₃. Physical Chemistry Chemical Physics, 2014, 16, 1424-1429.	1.3	306
53	How Many-Body Effects Modify the van der Waals Interaction between Graphene Sheets. Physical Review X, 2014, 4, .	2.8	35
54	The flexible nature of exchange, correlation, and Hartree physics: Resolving â€œdelocalizationâ€•errors in a â€œcorrelation freeâ€•density functional. Journal of Chemical Physics, 2013, 138, 014103.	1.2	37

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55	Electron affinities and ionisation potentials for atoms via â€œbenchmarkâ€•tdDFT calculations with and without exchange kernels. Journal of Chemical Physics, 2013, 138, 014109.	1.2	12
56	Assessment of range-separated time-dependent density-functional theory for calculating C6 dispersion coefficients. Journal of Chemical Physics, 2013, 138, 194106.	1.2	20
57	Dispersion corrections in graphenic systems: a simple and effective model of binding. Journal of Physics Condensed Matter, 2013, 25, 445010.	0.7	31
58	Effects of a finite Dirac cone on the dispersion properties of graphite. Physical Review B, 2013, 87, .	1.1	15
59	Binding and interlayer force in the near-contact region of two graphite slabs: Experiment and theory. Journal of Chemical Physics, 2013, 139, 224704.	1.2	21
60	Communication: Beyond the random phase approximation on the cheap: Improved correlation energies with the efficient â€œradial exchange holeâ€•kernel. Journal of Chemical Physics, 2012, 137, 111101.	1.2	31
61	Correlation energies beyond the random-phase approximation: Inhomogeneous Singwi-Tosi-Land-Sjolander functional applied to spherical atoms and ions. Physical Review A, 2012, 85, .	1.0	20
62	Calculation of dispersion energies. Journal of Physics Condensed Matter, 2012, 24, 073201.	0.7	187
63	Quantum continuum mechanics made simple. Journal of Chemical Physics, 2012, 136, 204115.	1.2	4
64	Efficient, long-range correlation from occupied wave functions only. Physical Review B, 2011, 84, .	1.1	8
65	Cohesive Properties and Asymptotics of the Dispersion Interaction in Graphite by the Random Phase Approximation. Physical Review Letters, 2010, 105, 196401.	2.9	330
66	van der Waals dispersion power laws for cleavage, exfoliation, and stretching in multiscale, layered systems. Physical Review B, 2009, 79, .	1.1	25
67	Dispersion interaction between crossed conducting wires. Physical Review A, 2009, 80, .	1.0	15
68	Theoretical and semiempirical correction to the long-range dispersion power law of stretched graphite. Physical Review B, 2008, 77, .	1.1	33
69	Dynamical model of Cosserat nanotubes. Journal of Physics: Conference Series, 2007, 62, 23-33.	0.3	3
70	A Cosserat rod model with microstructure. New Journal of Physics, 2006, 8, 137-137.	1.2	14
71	MEMS beams with defects: a model of non-ideal rods using a Cosserat approach for component level modelling. Journal of Micromechanics and Microengineering, 2005, 15, 76-80.	1.5	4
72	Correlation energies of inhomogeneous many-electron systems. Physical Review B, 2002, 66, .	1.1	55

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73	Prediction of Dispersion Forces: Is There a Problem?. Australian Journal of Chemistry, 2001, 54, 513.	0.5	148
74	A Novel Constraint for the Simplified Description of Dispersion Forces. Australian Journal of Physics, 2000, 53, 575.	0.6	6