Gino A Dilabio

List of Publications by Year
in descending order

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63	4,768	186265	110387
papers	citations	28 h-index	64 g-index

69	69	69	4974
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Predicting the Activity of Phenolic Antioxidants:Â Theoretical Method, Analysis of Substituent Effects, and Application to Major Families of Antioxidants. Journal of the American Chemical Society, 2001, 123, 1173-1183.	13.7	1,367
2	Dispersion interactions in densityâ€functional theory. Journal of Physical Organic Chemistry, 2009, 22, 1127-1135.	1.9	322
3	Field regulation of single-molecule conductivity by a charged surface atom. Nature, 2005, 435, 658-661.	27.8	289
4	Lone Pairâ€Ï€ and Ï€â€Ï€ Interactions Play an Important Role in Proton-Coupled Electron Transfer Reactions. Journal of the American Chemical Society, 2007, 129, 6199-6203.	13.7	185
5	Reaction of Phenols with the 2,2-Diphenyl-1-picrylhydrazyl Radical. Kinetics and DFT Calculations Applied To Determine ArO-H Bond Dissociation Enthalpies and Reaction Mechanism. Journal of Organic Chemistry, 2008, 73, 9270-9282.	3.2	148
6	Simple one-electron quantum capping potentials for use in hybrid QM/MM studies of biological molecules. Journal of Chemical Physics, 2002, 116, 9578-9584.	3.0	143
7	Patterning of Vinylferrocene on Hâ€Si(100) via Self-Directed Growth of Molecular Lines and STM-Induced Decomposition. Nano Letters, 2002, 2, 807-810.	9.1	139
8	Interactions in Large, Polyaromatic Hydrocarbon Dimers: Application of Density Functional Theory with Dispersion Corrections. Journal of Physical Chemistry A, 2008, 112, 10968-10976.	2.5	136
9	Bond Strengths of Toluenes, Anilines, and Phenols:â€‰ To Hammett or Not. Accounts of Chemical Research, 2004, 37, 334-340.	15.6	132
10	A (Nearly) Universally Applicable Method for Modeling Noncovalent Interactions Using B3LYP. Journal of Physical Chemistry Letters, 2012, 3, 1738-1744.	4.6	132
11	Performance of conventional and dispersion-corrected density-functional theory methods for hydrogen bonding interaction energies. Physical Chemistry Chemical Physics, 2013, 15, 12821.	2.8	120
12	The Unusual Reaction of Semiquinone Radicals with Molecular Oxygen. Journal of Organic Chemistry, 2008, 73, 1830-1841.	3.2	117
13	Density Functional Theory Based Model Calculations for Accurate Bond Dissociation Enthalpies. 3. A Single Approach for Xâ€H, Xâ€X, and Xâ€Y (X, Y = C, N, O, S, Halogen) Bonds. Journal of Physical Chemistry A, 2003, 107, 9953-9963.	2.5	109
14	Accurate treatment of van der Waals interactions using standard density functional theory methods with effective core-type potentials: Application to carbon-containing dimers. Chemical Physics Letters, 2008, 455, 348-353.	2.6	101
15	Halogen Bonding from Dispersion-Corrected Density-Functional Theory: The Role of Delocalization Error. Journal of Chemical Theory and Computation, 2014, 10, 5436-5447.	5.3	100
16	The Effect of Ring Nitrogen Atoms on the Homolytic Reactivity of Phenolic Compounds: Understanding the Radical-Scavenging Ability of 5-Pyrimidinols. Chemistry - A European Journal, 2003, 9, 4997-5010.	3.3	94
17	Approximations to complete basis set-extrapolated, highly correlated non-covalent interaction energies. Journal of Chemical Physics, 2011, 135, 134318.	3.0	81
18	A Theoretical Study of the Iminoxyl/Oxime Self-Exchange Reaction. A Five-Center, Cyclic Proton-Coupled Electron Transfer. Journal of the American Chemical Society, 2005, 127, 6693-6699.	13.7	73

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19	Accurate dispersion interactions from standard density-functional theory methods with small basis sets. Physical Chemistry Chemical Physics, 2010, 12, 6092.	2.8	52
20	Hydrogen Atom Abstraction Selectivity in the Reactions of Alkylamines with the Benzyloxyl and Cumyloxyl Radicals. The Importance of Structure and of Substrate Radical Hydrogen Bonding. Journal of the American Chemical Society, 2011, 133, 16625-16634.	13.7	49
21	Extension of the B3LYPâ€“dispersion-correcting potential approach to the accurate treatment of both inter- and intra-molecular interactions. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	45
22	Bimodal Evansâ€“Polanyi Relationships in Hydrogen Atom Transfer from C(sp³)â€“H Bonds to the Cumyloxyl Radical. A Combined Time-Resolved Kinetic and Computational Study. Journal of the American Chemical Society, 2021, 143, 11759-11776.	13.7	39
23	A Self-Directed Growth Process for Creating Covalently Bonded Molecular Assemblies on the Hâ^Si(100)-3Ã—1 Surface. Nano Letters, 2004, 4, 979-983.	9.1	38
24	Structureâ€“function relationships in aryl diazirines reveal optimal design features to maximize Câ€“H insertion. Chemical Science, 2021, 12, 12138-12148.	7.4	37
25	Extremely Fast Hydrogen Atom Transfer between Nitroxides and HOOÂ· Radicals and Implication for Catalytic Coantioxidant Systems. Journal of the American Chemical Society, 2018, 140, 10354-10362.	13.7	34
26	CO₂adsorption by nitrogen-doped carbon nanotubes predicted by density-functional theory with dispersion-correcting potentials. Physical Chemistry Chemical Physics, 2011, 13, 2780-2787.	2.8	31
27	Separability of spinâ€“orbit and correlation energies for the sixth-row main group hydride ground states. Journal of Chemical Physics, 1998, 108, 7527-7533.	3.0	30
28	Efficient basis sets for non-covalent interactions in XDM-corrected density-functional theory. Journal of Chemical Physics, 2013, 139, 214109.	3.0	29
29	Transferable Atom-Centered Potentials for the Correction of Basis Set Incompleteness Errors in Density-Functional Theory. Journal of Chemical Theory and Computation, 2017, 13, 3505-3524.	5.3	29
30	Detailed characterization of glycosylated sensory-active volatile phenols in smoke-exposed grapes and wine. Food Chemistry, 2018, 259, 147-156.	8.2	29
31	Importance of Ï€-Stacking Interactions in the Hydrogen Atom Transfer Reactions from Activated Phenols to Short-Lived N-Oxyl Radicals. Journal of Organic Chemistry, 2014, 79, 5209-5218.	3.2	28
32	Antioxidant activity of highly hydroxylated fullerene C60 and its interactions with the analogue of Î±-tocopherol. Free Radical Biology and Medicine, 2020, 160, 734-744.	2.9	28
33	Hydrogen Atom Abstraction Reactions from Tertiary Amines by Benzyloxyl and Cumyloxyl Radicals: Influence of Structure on the Rate-Determining Formation of a Hydrogen-Bonded Prereaction Complex. Journal of Organic Chemistry, 2011, 76, 6264-6270.	3.2	27
34	Reactions of the Cumyloxyl and Benzyloxyl Radicals with Strong Hydrogen Bond Acceptors. Large Enhancements in Hydrogen Abstraction Reactivity Determined by Substrate/Radical Hydrogen Bonding. Journal of Organic Chemistry, 2012, 77, 10479-10487.	3.2	27
35	Dispersion Corrections Improve the Accuracy of Both Noncovalent and Covalent Interactions Energies Predicted by a Density-Functional Theory Approximation. Journal of Physical Chemistry A, 2015, 119, 6703-6713.	2.5	27
36	Flexible polyfluorinated bis-diazirines as molecular adhesives. Chemical Science, 2021, 12, 4147-4153.	7.4	27

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37	BH9, a New Comprehensive Benchmark Data Set for Barrier Heights and Reaction Energies: Assessment of Density Functional Approximations and Basis Set Incompleteness Potentials. Journal of Chemical Theory and Computation, 2022, 18, 151-166.	5.3	27
38	Reactions of the Phthalimide N-Oxyl Radical (PINO) with Activated Phenols: The Contribution of Ï€-Stacking Interactions to Hydrogen Atom Transfer Rates. Journal of Organic Chemistry, 2013, 78, 1026-1037.	3.2	25
39	Hydrogen Atom Transfer (HAT) Processes Promoted by the Quinolinimide-N-oxyl Radical. A Kinetic and Theoretical Study. Journal of Organic Chemistry, 2017, 82, 6133-6141.	3.2	25
40	Exchangeâ€“Correlation Effects for Noncovalent Interactions in Density Functional Theory. Journal of Chemical Theory and Computation, 2016, 12, 3160-3175.	5.3	24
41	Dispersion-correcting potentials can significantly improve the bond dissociation enthalpies and noncovalent binding energies predicted by density-functional theory. Journal of Chemical Physics, 2014, 140, 18A542.	3.0	23
42	PEPCONF, a diverse data set of peptide conformational energies. Scientific Data, 2019, 6, 180310.	5.3	23
43	Are we failing female and racialized academics? A Canadian national survey examining the impacts of the COVIDâ€19 pandemic on tenure and tenureâ€track faculty. Gender, Work and Organization, 2022, 29, 703-722.	4.7	23
44	Atom-Centered Potentials with Dispersion-Corrected Minimal-Basis-Set Hartreeâ€“Fock: An Efficient and Accurate Computational Approach for Large Molecular Systems. Journal of Chemical Theory and Computation, 2018, 14, 726-738.	5.3	18
45	Evaluation of Polar Effects in Hydrogen Atom Transfer Reactions from Activated Phenols. Journal of Organic Chemistry, 2019, 84, 1778-1786.	3.2	16
46	Improved Basis-Set Incompleteness Potentials for Accurate Density-Functional Theory Calculations in Large Systems. Journal of Chemical Theory and Computation, 2020, 16, 4176-4191.	5.3	15
47	Pentacene Binds Strongly to Hydrogen-Terminated Silicon Surfaces Via Dispersion Interactions. Journal of Physical Chemistry C, 2009, 113, 9969-9973.	3.1	12
48	Density-Functional Theory with Dispersion-Correcting Potentials for Methane: Bridging the Efficiency and Accuracy Gap between High-Level Wave Function and Classical Molecular Mechanics Methods. Journal of Chemical Theory and Computation, 2013, 9, 3342-3349.	5.3	12
49	A Meta Effect in Nonphotochemical Processes:â€‰ The Homolytic Chemistry of m-Methoxyphenol. Journal of Organic Chemistry, 2008, 73, 2408-2411.	3.2	11
50	Accurate Modeling of Water Clusters with Density-Functional Theory Using Atom-Centered Potentials. Journal of Chemical Theory and Computation, 2017, 13, 4205-4215.	5.3	10
51	Computational Study of Hydrogen Bond Interactions in Water Clusterâ€“Organic Molecule Complexes. Journal of Physical Chemistry A, 2021, 125, 3369-3377.	2.5	10
52	BSE49, a diverse, high-quality benchmark dataset of separation energies of chemical bonds. Scientific Data, 2021, 8, 300.	5.3	9
53	Extent of conjugation in diazonium-derived layers in molecular junction devices determined by experiment and modelling. Physical Chemistry Chemical Physics, 2019, 21, 16762-16770.	2.8	8
54	Fast and Accurate Quantum Mechanical Modeling of Large Molecular Systems Using Small Basis Set Hartreeâ€“Fock Methods Corrected with Atom-Centered Potentials. Journal of Chemical Theory and Computation, 2022, 18, 2208-2232.	5.3	7

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55	Performance of small basis set Hartreeâ€“Fock methods for modeling non-covalent interactions. Electronic Structure, 2021, 3, 034007.	2.8	6
56	Influence of Topical Cross-Linking on Mechanical and Ballistic Performance of a Woven Ultra-High-Molecular-Weight Polyethylene Fabric Used in Soft Body Armor. ACS Applied Polymer Materials, 2021, 3, 6008-6018.	4.4	6
57	Ring-opening radical clock reactions: many density functionals have difficulty keeping time. Organic and Biomolecular Chemistry, 2011, 9, 3158.	2.8	5
58	Kinetics of the Addition of Olefins to Si-Centered Radicals: The Critical Role of Dispersion Interactions Revealed by Theory and Experiment. Journal of Physical Chemistry A, 2015, 119, 5883-5888.	2.5	5
59	Ab initio characterization of coupling strength for all types of dangling-bond pairs on the hydrogen-terminated Si(100)-2 Ã— 1 surface. Journal of Chemical Physics, 2018, 148, 154701.	3.0	4
60	Small-Basis Set Density-Functional Theory Methods Corrected with Atom-Centered Potentials. Journal of Chemical Theory and Computation, 2022, 18, 2913-2930.	5.3	4
61	Atom-Centered Potentials for Noncovalent Interactions and Other Applications. , 2017, , 221-240.		3
62	Reply to the â€˜Comment on â€œExtent of conjugation in diazonium-derived layers in molecular junction devices determined by experiment and modellingâ€â€™ by R. L. McCreery, S. K. Saxena, M. Supur and U. Tefashe, Phys. Chem. Chem. Phys., 2020, 22, DOI: 10.1039/d0cp02412k. Physical Chemistry Chemical Physics, 2020, 22, 21547-21549.	2.8	2
63	Dramatic relativistic and magnetic Breit effects for the superheavy reaction Ogâ€‰+â€‰3Ts2â€‰â†’â€‰OgTs6: prediction of atomization energy and the existence of the superheavy octahedral oganesson hexatennesside OgTs6. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	1