Pavlo O Dral

List of Publications by Year
in descending order

43	3,316	279798 23	265206 42
papers	citations	h-index	g-index

44	44	44	3109
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantum chemistry structures and properties of 134 kilo molecules. Scientific Data, 2014, 1, 140022.	5.3	887
2	Big Data Meets Quantum Chemistry Approximations: The Î”-Machine Learning Approach. Journal of Chemical Theory and Computation, 2015, 11, 2087-2096.	5.3	579
3	Quantum Chemistry in the Age of Machine Learning. Journal of Physical Chemistry Letters, 2020, 11, 2336-2347.	4.6	258
4	Deep Learning for Nonadiabatic Excited-State Dynamics. Journal of Physical Chemistry Letters, 2018, 9, 6702-6708.	4.6	126
5	Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Theory, Implementation, and Parameters. Journal of Chemical Theory and Computation, 2016, 12, 1082-1096.	5.3	123
6	Nonadiabatic Excited-State Dynamics with Machine Learning. Journal of Physical Chemistry Letters, 2018, 9, 5660-5663.	4.6	116
7	Molecular excited states through a machine learning lens. Nature Reviews Chemistry, 2021, 5, 388-405.	30.2	107
8	Structure-based sampling and self-correcting machine learning for accurate calculations of potential energy surfaces and vibrational levels. Journal of Chemical Physics, 2017, 146, 244108.	3.0	106
9	The Relationship between Threshold Voltage and Dipolar Character of Self-Assembled Monolayers in Organic Thin-Film Transistors. Journal of the American Chemical Society, 2012, 134, 12648-12652.	13.7	88
10	Machine Learning of Parameters for Accurate Semiempirical Quantum Chemical Calculations. Journal of Chemical Theory and Computation, 2015, 11, 2120-2125.	5.3	86
11	Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Benchmarks for Ground-State Properties. Journal of Chemical Theory and Computation, 2016, 12, 1097-1120.	5.3	74
12	Choosing the right molecular machine learning potential. Chemical Science, 2021, 12, 14396-14413.	7.4	72
13	Hierarchical machine learning of potential energy surfaces. Journal of Chemical Physics, 2020, 152, 204110.	3.0	57
14	Artificial intelligence-enhanced quantum chemical method with broad applicability. Nature Communications, 2021, 12, 7022.	12.8	52
15	MLatom: A program package for quantum chemical research assisted by machine learning. Journal of Computational Chemistry, 2019, 40, 2339-2347.	3.3	51
16	Oxygen-Doped Nanodiamonds: Synthesis and Functionalizations. Organic Letters, 2009, 11, 3068-3071.	4.6	50
17	Machine Learning for Absorption Cross Sections. Journal of Physical Chemistry A, 2020, 124, 7199-7210.	2.5	50
18	Semiempirical Quantum-Chemical Methods with Orthogonalization and Dispersion Corrections. Journal of Chemical Theory and Computation, 2019, 15, 1743-1760.	5.3	45

#	Article	IF	Citations
19	MLatom 2: An Integrative Platform for Atomistic Machine Learning. Topics in Current Chemistry, 2021, 379, 27.	5.8	38
20	Doped Polycyclic Aromatic Hydrocarbons as Building Blocks for Nanoelectronics: A Theoretical Study. Journal of Organic Chemistry, 2013, 78, 1894-1902.	3.2	32
21	Semiempirical UNOâ€“CAS and UNOâ€“CI: Method and Applications in Nanoelectronics. Journal of Physical Chemistry A, 2011, 115, 11303-11312.	2.5	30
22	Configurationally Stable Chiral Dithiaâ€Bridged Hetero[4]helicene Radical Cation: Electronic Structure and Absolute Configuration. Chemistry - an Asian Journal, 2017, 12, 31-35.	3.3	29
23	Organic Electron Acceptors Comprising a Dicyanomethyleneâ€Bridged Acridophosphine Scaffold: The Impact of the Heteroatom. Chemistry - A European Journal, 2017, 23, 6988-6992.	3.3	28
24	Calculating distribution coefficients based on multi-scale free energy simulations: an evaluation of MM and QM/MM explicit solvent simulations of water-cyclohexane transfer in the SAMPL5 challenge. Journal of Computer-Aided Molecular Design, 2016, 30, 989-1006.	2.9	24
25	A Ïâ€Stacked Porphyrinâ€“Fullerene Electron Donorâ€“Acceptor Conjugate That Features a Surprising Frozen Geometry. Chemistry - A European Journal, 2012, 18, 14008-14016.	3.3	23
26	A Spherically Shielded Triphenylamine and Its Persistent Radical Cation. Chemistry - A European Journal, 2020, 26, 3264-3269.	3.3	23
27	Toward Chemical Accuracy in Predicting Enthalpies of Formation with General-Purpose Data-Driven Methods. Journal of Physical Chemistry Letters, 2022, 13, 3479-3491.	4.6	22
28	Predicting the future of excitation energy transfer in light-harvesting complex with artificial intelligence-based quantum dynamics. Nature Communications, 2022, 13, 1930.	12.8	21
29	Multiply Bonded Metal(II) Acetate (Rhodium, Ruthenium, and Molybdenum) Complexes with the trans-1,2-Bis(N-methylimidazol-2-yl)ethylene Ligand. Inorganic Chemistry, 2014, 53, 12305-12314.	4.0	20
30	N-Heterotriangulene chromophores with 4-pyridyl anchors for dye-sensitized solar cells. RSC Advances, 2016, 6, 67372-67377.	3.6	20
31	Big data analysis of ab Initio molecular integrals in the neglect of diatomic differential overlap approximation. Journal of Computational Chemistry, 2019, 40, 638-649.	3.3	10
32	What is semiempirical molecular orbital theory approximating?. Journal of Molecular Modeling, 2019, 25, 119.	1.8	10
33	The Impact of Aggregation on the Photophysics of Spiroâ€Bridged Heterotriangulenes. Angewandte Chemie - International Edition, 2020, 59, 16233-16240.	13.8	10
34	Probing Charge Transfer in Benzodifuranâ€“C₆₀ Dumbbellâ€Type Electron Donorâ€“Acceptor Conjugates: Groundâ€and Excitedâ€State Assays. ChemPhysChem, 2013, 14, 2910-2919.	2.1	9
35	Stability of Oddâ€Versus Evenâ€Electron Gasâ€Phase (Quasi)Molecular Ions Derived from Pyridineâ€Substituted Nâ€Heterotriangulenes. ChemPlusChem, 2017, 82, 204-211.	2.8	9
36	Dithiafulvenylâ€Extended Nâ€Heterotriangulenes and Their Interaction with C₆₀: Cooperative Fluorescence. Chemistry - A European Journal, 2017, 23, 12353-12362.	3.3	8

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37	Influence of Electron Doping on the Hydrogenation of Fullerene C₆₀: A Theoretical Investigation. ChemPhysChem, 2011, 12, 2581-2589.	2.1	4
38	The unrestricted local properties: application in nanoelectronics and for predicting radicals reactivity. Journal of Molecular Modeling, 2014, 20, 2134.	1.8	4
39	On the feasibility of reactions through the fullerene wall: a theoretical study of NH_x@C₆₀. Physical Chemistry Chemical Physics, 2017, 19, 17199-17209.	2.8	4
40	1D Chains of Diruthenium Tetracarbonyl Sawhorse Complexes. European Journal of Inorganic Chemistry, 2018, 2018, 54-61.	2.0	4
41	5,7,12,14-Tetraphenyl-Substituted 6,13-Diazapentacenes as Versatile Organic Semiconductors: Characterization in Field Effect Transistors. Organic Materials, 2020, 02, 204-213.	2.0	4
42	VIB5 database with accurate ab initio quantum chemical molecular potential energy surfaces. Scientific Data, 2022, 9, 84.	5.3	3
43	Stability of Odd- Versus Even-Electron Gas-Phase (Quasi)Molecular Ions Derived from Pyridine-Substituted N-Heterotriangulenes. ChemPlusChem, 2017, 82, 163-163.	2.8	0