Pavlo O Dral

List of Publications by Year
in descending order

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43 papers	3,316 citations	279798 23 h-index	265206 42 g-index
44 all docs	44 docs citations	44 times ranked	3109 citing authors

#	Article	IF	Citations
1	VIB5 database with accurate ab initio quantum chemical molecular potential energy surfaces. Scientific Data, 2022, 9, 84.	5.3	3
2	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
3	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
4	Choosing the right molecular machine learning potential. Chemical Science, 2021, 12, 14396-14413.	7.4	72
5	Molecular excited states through a machine learning lens. Nature Reviews Chemistry, 2021, 5, 388-405.	30.2	107
6	MLatom 2: An Integrative Platform for Atomistic Machine Learning. Topics in Current Chemistry, 2021, 379, 27.	5.8	38
7	Artificial intelligence-enhanced quantum chemical method with broad applicability. Nature Communications, 2021, 12, 7022.	12.8	52
8	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
9	Machine Learning for Absorption Cross Sections. Journal of Physical Chemistry A, 2020, 124, 7199-7210.	2.5	50
10	The Impact of Aggregation on the Photophysics of Spiroâ€Bridged Heterotriangulenes. Angewandte Chemie - International Edition, 2020, 59, 16233-16240.	13.8	10
11	Hierarchical machine learning of potential energy surfaces. Journal of Chemical Physics, 2020, 152, 204110.	3.0	57
12	Quantum Chemistry in the Age of Machine Learning. Journal of Physical Chemistry Letters, 2020, 11, 2336-2347.	4.6	258
13	A Spherically Shielded Triphenylamine and Its Persistent Radical Cation. Chemistry - A European Journal, 2020, 26, 3264-3269.	3.3	23
14	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
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	What is semiempirical molecular orbital theory approximating?. Journal of Molecular Modeling, 2019, 25, 119.	1.8	10
17	Semiempirical Quantum-Chemical Methods with Orthogonalization and Dispersion Corrections. Journal of Chemical Theory and Computation, 2019, 15, 1743-1760.	5.3	45
18	1D Chains of Diruthenium Tetracarbonyl Sawhorse Complexes. European Journal of Inorganic Chemistry, 2018, 2018, 54-61.	2.0	4

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19	Deep Learning for Nonadiabatic Excited-State Dynamics. Journal of Physical Chemistry Letters, 2018, 9, 6702-6708.	4.6	126
20	Nonadiabatic Excited-State Dynamics with Machine Learning. Journal of Physical Chemistry Letters, 2018, 9, 5660-5663.	4.6	116
21	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
22	Dithiafulvenylâ€Extended Nâ€Heterotriangulenes and Their Interaction with C₆₀: Cooperative Fluorescence. Chemistry - A European Journal, 2017, 23, 12353-12362.	3.3	8
23	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
24	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
25	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
26	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
27	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
28	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
29	N-Heterotriangulene chromophores with 4-pyridyl anchors for dye-sensitized solar cells. RSC Advances, 2016, 6, 67372-67377.	3.6	20
30	Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Theory, Implementation, and Parameters. Journal of Chemical Theory and Computation, 2016, 12, 1082-1096.	5.3	123
31	Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Benchmarks for Ground-State Properties. Journal of Chemical Theory and Computation, 2016, 12, 1097-1120.	5.3	74
32	Machine Learning of Parameters for Accurate Semiempirical Quantum Chemical Calculations. Journal of Chemical Theory and Computation, 2015, 11, 2120-2125.	5.3	86
33	Big Data Meets Quantum Chemistry Approximations: The Î”-Machine Learning Approach. Journal of Chemical Theory and Computation, 2015, 11, 2087-2096.	5.3	579
34	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
35	The unrestricted local properties: application in nanoelectronics and for predicting radicals reactivity. Journal of Molecular Modeling, 2014, 20, 2134.	1.8	4
36	Quantum chemistry structures and properties of 134 kilo molecules. Scientific Data, 2014, 1, 140022.	5.3	887

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37	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
38	Doped Polycyclic Aromatic Hydrocarbons as Building Blocks for Nanoelectronics: A Theoretical Study. Journal of Organic Chemistry, 2013, 78, 1894-1902.	3.2	32
39	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
40	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
41	Semiempirical UNOâ€“CAS and UNOâ€“CI: Method and Applications in Nanoelectronics. Journal of Physical Chemistry A, 2011, 115, 11303-11312.	2.5	30
42	Influence of Electron Doping on the Hydrogenation of Fullerene C₆₀: A Theoretical Investigation. ChemPhysChem, 2011, 12, 2581-2589.	2.1	4
43	Oxygen-Doped Nanodiamonds: Synthesis and Functionalizations. Organic Letters, 2009, 11, 3068-3071.	4.6	50