Art D Bochevarov

List of Publications by Year
in descending order

22 papers	2,209 citations	623734 14 h-index	677142 22 g-index
22 all docs	22 docs citations	22 times ranked	3911 citing authors

#	Article	IF	Citations
1	Jaguar: A highâ€performance quantum chemistry software program with strengths in life and materials sciences. International Journal of Quantum Chemistry, 2013, 113, 2110-2142.	2.0	1,426
2	Automated Transition State Search and Its Application to Diverse Types of Organic Reactions. Journal of Chemical Theory and Computation, 2017, 13, 5780-5797.	5.3	125
3	Multiconformation, Density Functional Theory-Based pK_a Prediction in Application to Large, Flexible Organic Molecules with Diverse Functional Groups. Journal of Chemical Theory and Computation, 2016, 12, 6001-6019.	5.3	108
4	Empirical Conversion of pK_a Values between Different Solvents and Interpretation of the Parameters: Application to Water, Acetonitrile, Dimethyl Sulfoxide, and Methanol. ACS Omega, 2018, 3, 1653-1662.	3.5	92
5	The electron and nuclear orbitals model: current challenges and future prospects. Molecular Physics, 2004, 102, 111-123.	1.7	84
6	Parameterization of a B3LYP Specific Correction for Noncovalent Interactions and Basis Set Superposition Error on a Gigantic Data Set of CCSD(T) Quality Noncovalent Interaction Energies. Journal of Chemical Theory and Computation, 2011, 7, 658-668.	5.3	73
7	Prediction of ⁵⁷Fe MÃ¶ssbauer Parameters by Density Functional Theory: A Benchmark Study. Journal of Chemical Theory and Computation, 2010, 6, 3735-3749.	5.3	54
8	Insights into the Different Dioxygen Activation Pathways of Methane and Toluene Monooxygenase Hydroxylases. Journal of the American Chemical Society, 2011, 133, 7384-7397.	13.7	45
9	Weighted Averaging Scheme and Local Atomic Descriptor for pK_a Prediction Based on Density Functional Theory. Journal of Chemical Information and Modeling, 2018, 58, 271-286.	5.4	33
10	The densities produced by the density functional theory: Comparison to full configuration interaction. Journal of Chemical Physics, 2008, 128, 034102.	3.0	30
11	Quantum chemical prediction for complex organic molecules. International Journal of Quantum Chemistry, 2018, 118, e25561.	2.0	24
12	Localized Orbital Corrections for the Barrier Heights in Density Functional Theory. Journal of Chemical Theory and Computation, 2009, 5, 2996-3009.	5.3	21
13	Hybrid correlation models based on active-space partitioning: Correcting second-order MÃllerâ€“Plesset perturbation theory for bond-breaking reactions. Journal of Chemical Physics, 2005, 122, 234110.	3.0	19
14	Localized orbital corrections applied to thermochemical errors in density functional theory: The role of basis set and application to molecular reactions. Journal of Chemical Physics, 2008, 129, 214105.	3.0	19
15	A general diagrammatic algorithm for contraction and subsequent simplification of second-quantized expressions. Journal of Chemical Physics, 2004, 121, 3374-3383.	3.0	12
16	Discovery of a Novel Class of <scp>d</scp>-Amino Acid Oxidase Inhibitors Using the SchrÃ¶dinger Computational Platform. Journal of Medicinal Chemistry, 2022, 65, 6775-6802.	6.4	10
17	Continuous Localized Orbital Corrections to Density Functional Theory: B3LYP-CLOC. Journal of Chemical Theory and Computation, 2010, 6, 3647-3663.	5.3	9
18	Generation of Tautomers Using Micro-pKaâ€™s. Journal of Chemical Information and Modeling, 2019, 59, 2672-2689.	5.4	8

#	Article	IF	Citations
19	Hybrid correlation models based on active-space partitioning: Seeking accurate O(N5) ab initio methods for bond breaking. Journal of Chemical Physics, 2006, 125, 054109.	3.0	7
20	Some Simple Results Following from LÃ¶wdinâ€™s Partitioning Technique. Journal of Mathematical Chemistry, 2007, 42, 59-64.	1.5	6
21	Accurate Quantum Chemical Calculation of Ionization Potentials: Validation of the DFT-LOC Approach via a Large Data Set Obtained from Experiments and Benchmark Quantum Chemical Calculations. Journal of Chemical Theory and Computation, 2020, 16, 2109-2123.	5.3	2
22	Pattern-free generation and quantumÂmechanical scoring of ring-chain tautomers. Journal of Computer-Aided Molecular Design, 2021, 35, 417-431.	2.9	2