

# Art D Bochevarov

## List of Publications by Year in descending order

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Version: 2024-02-01

22  
papers

2,209  
citations

623188

14  
h-index

676716

22  
g-index

22  
all docs

22  
docs citations

22  
times ranked

3911  
citing authors

#	ARTICLE	IF	CITATIONS
1	Discovery of a Novel Class of $\alpha$ -Amino Acid Oxidase Inhibitors Using the Schrödinger Computational Platform. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 6775-6802.	2.9	10
2	Pattern-free generation and quantum-mechanical scoring of ring-chain tautomers. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 417-431.	1.3	2
3	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. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2109-2123.	2.3	2
4	Generation of Tautomers Using Micro-pKa <sup>TM</sup> s. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2672-2689.	2.5	8
5	Empirical Conversion of $pK_a$ Values between Different Solvents and Interpretation of the Parameters: Application to Water, Acetonitrile, Dimethyl Sulfoxide, and Methanol. <i>ACS Omega</i> , 2018, 3, 1653-1662.	1.6	92
6	Weighted Averaging Scheme and Local Atomic Descriptor for $pK_a$ Prediction Based on Density Functional Theory. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 271-286.	2.5	33
7	Quantum chemical prediction for complex organic molecules. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25561.	1.0	24
8	Automated Transition State Search and Its Application to Diverse Types of Organic Reactions. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5780-5797.	2.3	125
9	Multiconformation, Density Functional Theory-Based $pK_a$ Prediction in Application to Large, Flexible Organic Molecules with Diverse Functional Groups. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 6001-6019.	2.3	108
10	Jaguar: A high-performance quantum chemistry software program with strengths in life and materials sciences. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2110-2142.	1.0	1,426
11	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. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 658-668.	2.3	73
12	Insights into the Different Dioxygen Activation Pathways of Methane and Toluene Monooxygenase Hydroxylases. <i>Journal of the American Chemical Society</i> , 2011, 133, 7384-7397.	6.6	45
13	Prediction of $^{57}\text{Fe}$ Mössbauer Parameters by Density Functional Theory: A Benchmark Study. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3735-3749.	2.3	54
14	Continuous Localized Orbital Corrections to Density Functional Theory: B3LYP-CLOC. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3647-3663.	2.3	9
15	Localized Orbital Corrections for the Barrier Heights in Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2996-3009.	2.3	21
16	The densities produced by the density functional theory: Comparison to full configuration interaction. <i>Journal of Chemical Physics</i> , 2008, 128, 034102.	1.2	30
17	Localized orbital corrections applied to thermochemical errors in density functional theory: The role of basis set and application to molecular reactions. <i>Journal of Chemical Physics</i> , 2008, 129, 214105.	1.2	19
18	Some Simple Results Following from Löwdin's Partitioning Technique. <i>Journal of Mathematical Chemistry</i> , 2007, 42, 59-64.	0.7	6

#	ARTICLE	IF	CITATIONS
19	Hybrid correlation models based on active-space partitioning: Seeking accurate O(N <sup>5</sup> ) ab initio methods for bond breaking. <i>Journal of Chemical Physics</i> , 2006, 125, 054109.	1.2	7
20	Hybrid correlation models based on active-space partitioning: Correcting second-order Møller-Plesset perturbation theory for bond-breaking reactions. <i>Journal of Chemical Physics</i> , 2005, 122, 234110.	1.2	19
21	The electron and nuclear orbitals model: current challenges and future prospects. <i>Molecular Physics</i> , 2004, 102, 111-123.	0.8	84
22	A general diagrammatic algorithm for contraction and subsequent simplification of second-quantized expressions. <i>Journal of Chemical Physics</i> , 2004, 121, 3374-3383.	1.2	12