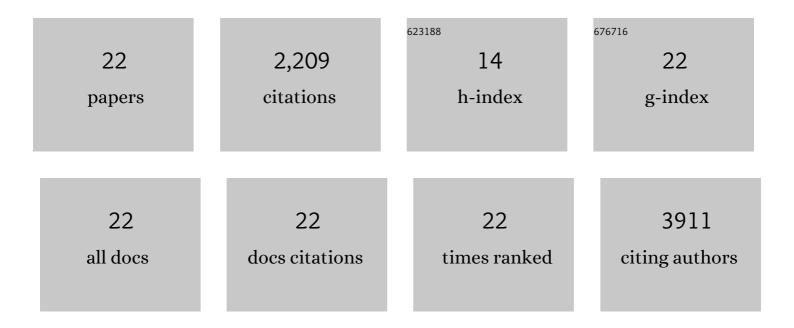
Art D Bochevarov

List of Publications by Year in descending order

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APT D ROCHEVAPOV

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

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#	Article	IF	CITATIONS
			Si Milons
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.	1.2	7
20	Hybrid correlation models based on active-space partitioning: Correcting second-order MÃ,ller–Plesset perturbation theory for bond-breaking reactions. Journal of Chemical Physics, 2005, 122, 234110.	1.2	19
21	The electron and nuclear orbitals model: current challenges and future prospects. Molecular Physics, 2004, 102, 111-123.	0.8	84
22	A general diagrammatic algorithm for contraction and subsequent simplification of second-quantized expressions. Journal of Chemical Physics, 2004, 121, 3374-3383.	1.2	12