Arkajyoti Sengupta

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7141573/publications.pdf

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22	812	567144 15	642610 23
papers	citations	h-index	g-index

25	25	25	891
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Anion Binding in Solution: Beyond the Electrostatic Regime. CheM, 2017, 3, 411-427.	5.8	129
2	Anions Stabilize Each Other inside Macrocyclic Hosts. Angewandte Chemie - International Edition, 2016, 55, 14057-14062.	7.2	115
3	Parameterization of Monovalent Ions for the OPC3, OPC, TIP3P-FB, and TIP4P-FB Water Models. Journal of Chemical Information and Modeling, 2021, 61, 869-880.	2.5	81
4	Electrostatic and Allosteric Cooperativity in Ion-Pair Binding: A Quantitative and Coupled Experimentâ€“Theory Study with Arylâ€“Triazoleâ€“Ether Macrocycles. Journal of the American Chemical Society, 2015, 137, 9746-9757.	6.6	69
5	Flexibility Coexists with Shape-Persistence in Cyanostar Macrocycles. Journal of the American Chemical Society, 2016, 138, 4843-4851.	6.6	53
6	An Enzymatic Platform for Primary Amination of 1-Aryl-2-alkyl Alkynes. Journal of the American Chemical Society, 2022, 144, 80-85.	6.6	41
7	Mechanistic Insights on Organocatalytic Enantioselective Decarboxylative Protonation by Epicinchona-Thiourea Hybrid Derivatives. Journal of Organic Chemistry, 2012, 77, 10525-10536.	1.7	30
8	Prediction of Accurate Thermochemistry of Medium and Large Sized Radicals Using Connectivity-Based Hierarchy (CBH). Journal of Chemical Theory and Computation, 2014, 10, 4342-4350.	2.3	30
9	Simulating the Chelate Effect. Journal of the American Chemical Society, 2018, 140, 15166-15169.	6.6	29
10	Thermodynamics of Transition Metal Ion Binding to Proteins. Journal of the American Chemical Society, 2020, 142, 6365-6374.	6.6	28
11	Application of the Generalized Connectivity-Based Hierarchy to Biomonomers: Enthalpies of Formation of Cysteine and Methionine. Journal of Physical Chemistry A, 2013, 117, 4973-4980.	1.1	27
12	Solving the Density Functional Conundrum: Elimination of Systematic Errors To Derive Accurate Reaction Enthalpies of Complex Organic Reactions. Organic Letters, 2017, 19, 2576-2579.	2.4	27
13	Anions Stabilize Each Other inside Macrocyclic Hosts. Angewandte Chemie, 2016, 128, 14263-14268.	1.6	25
14	Anionâ€Binding Macrocycles Operate Beyond the Electrostatic Regime: Interaction Distances Matter. Chemistry - A European Journal, 2018, 24, 14409-14417.	1.7	20
15	Cycloadditions of Cyclopentadiene and Cycloheptatriene with Tropones: All Endo-[6+4] Cycloadditions Are Ambimodal. Journal of the American Chemical Society, 2021, 143, 3918-3926.	6.6	20
16	Eliminating Systematic Errors in DFT via Connectivity-Based Hierarchy: Accurate Bond Dissociation Energies of Biodiesel Methyl Esters. Journal of Physical Chemistry A, 2019, 123, 3543-3550.	1.1	14
17	Accurate and Computationally Efficient Prediction of Thermochemical Properties of Biomolecules Using the Generalized Connectivity-Based Hierarchy. Journal of Physical Chemistry B, 2014, 118, 9631-9643.	1.2	13
18	Direct Reduction of Alkyl Monohalides at Silver in Dimethylformamide: Effects of Position and Identity of the Halogen. ChemElectroChem, 2015, 2, 726-736.	1.7	13

#	Article	IF	Citations
19	Accurate Thermochemistry for Organic Cations via Error Cancellation using Connectivity-Based Hierarchy. Journal of Physical Chemistry A, 2018, 122, 1807-1812.	1.1	12
20	Fragment-Based Approaches for Supramolecular Interaction Energies: Applications to Foldamers and Their Complexes with Anions. Journal of Chemical Theory and Computation, 2018, 14, 6226-6239.	2.3	12
21	Electrochemical reduction of 2-chloro-N-phenylacetamides at carbon and silver cathodes in dimethylformamide. Electrochimica Acta, 2014, 127, 159-166.	2.6	11
22	Breaking a bottleneck: Accurate extrapolation to â€œgold standardâ€•CCSD(T) energies for large open shell organic radicals at reduced computational cost. Journal of Computational Chemistry, 2016, 37, 286-295.	1.5	6