Rebecca Sure

List of Publications by Year
in descending order

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21 papers	1,535 citations	393982 19 h-index	676716 22 g-index
24 all docs	24 docs citations	24 times ranked	2092 citing authors

#	Article	IF	Citations
1	Towards a converged strategy for including microsolvation in reaction mechanism calculations. Journal of Computer-Aided Molecular Design, 2021, 35, 473-492.	1.3	23
2	Bismuth as a versatile cation for luminescence in coordination polymers from BiX₃/4,4â€²-bipy: understanding of photophysics by quantum chemical calculations and structural parallels to lanthanides. Dalton Transactions, 2018, 47, 7669-7681.	1.6	43
3	Comprehensive theoretical study of all 1812 C₆₀ isomers. Physical Chemistry Chemical Physics, 2017, 19, 14296-14305.	1.3	58
4	Quantum Chemical Dissection of the Shortest P=Oâ‹…â‹…â‹…I Halogen Bond: The Decisive Role of Crystal Packing Effects. Chemistry - A European Journal, 2017, 23, 5687-5691.	1.7	20
5	HYDROPHOBE Challenge: A Joint Experimental and Computational Study on the Hostâ€“Guest Binding of Hydrocarbons to Cucurbiturils, Allowing Explicit Evaluation of Guest Hydration Free-Energy Contributions. Journal of Physical Chemistry B, 2017, 121, 11144-11162.	1.2	62
6	Halogen bonded supramolecular capsules: a challenging test case for quantum chemical methods. Chemical Communications, 2016, 52, 9893-9896.	2.2	26
7	Hochaktive Titanocenâ€Katalysatoren fÃ¼r Epoxidâ€Hydrosilylierungen â€“ Synthese, Theorie, Kinetik, EPRâ€Spektroskopie. Angewandte Chemie, 2016, 128, 7801-7805.	1.6	27
8	From small fullerenes to the graphene limit: A harmonic forceâ€field method for fullerenes and a comparison to density functional calculations for <scp>G</scp>oldbergâ€“<scp>C</scp>oxeter fullerenes up to C₉₈₀. Journal of Computational Chemistry, 2016, 37, 10-17.	1.5	12
9	Small Atomic Orbital Basis Set Firstâ€Principles Quantum Chemical Methods for Large Molecular and Periodic Systems: A Critical Analysis of Error Sources. ChemistryOpen, 2016, 5, 94-109.	0.9	57
10	Highly Active Titanocene Catalysts for Epoxide Hydrosilylation: Synthesis, Theory, Kinetics, EPR Spectroscopy. Angewandte Chemie - International Edition, 2016, 55, 7671-7675.	7.2	57
11	Comprehensive Benchmark of Association (Free) Energies of Realistic Hostâ€“Guest Complexes. Journal of Chemical Theory and Computation, 2015, 11, 3785-3801.	2.3	188
12	A systematic study of rare gas atoms encapsulated in small fullerenes using dispersion corrected density functional theory. Journal of Computational Chemistry, 2015, 36, 88-96.	1.5	28
13	Using dispersion-corrected density functional theory to understand supramolecular binding thermodynamics. Chemical Communications, 2015, 51, 1764-1774.	2.2	125
14	Mechanistic Study of the Titanocene(III)â€Catalyzed Radical Arylation of Epoxides. Chemistry - A European Journal, 2015, 21, 280-289.	1.7	71
15	Blind Prediction of Binding Affinities for Charged Supramolecular Hostâ€“Guest Systems: Achievements and Shortcomings of DFT-D3. Journal of Physical Chemistry B, 2014, 118, 3431-3440.	1.2	77
16	Substituent Effects and Supramolecular Interactions of Titanocene(III) Chloride: Implications for Catalysis in Single Electron Steps. Journal of the American Chemical Society, 2014, 136, 1663-1671.	6.6	78
17	Synthesis, Chiral Resolution, and Absolute Configuration of Dissymmetric 4,15-Difunctionalized [2.2]Paracyclophanes. Journal of Organic Chemistry, 2014, 79, 6679-6687.	1.7	33
18	Nearly Degenerate Isomers of C(BH)₂: Cumulene, Carbene, or Carbone?. Chemistry - A European Journal, 2013, 19, 15941-15954.	1.7	25

#	Article	IF	Citations
19	Corrected small basis set Hartreeâ€Fock method for large systems. Journal of Computational Chemistry, 2013, 34, 1672-1685.	1.5	358
20	Computational study of the rate constants and free energies of intramolecular radical addition to substituted anilines. Beilstein Journal of Organic Chemistry, 2013, 9, 1620-1629.	1.3	27
21	Borylene Complexes (BH)L₂ and Nitrogen Cation Complexes (N⁺)L₂: Isoelectronic Homologues of Carbones CL₂. Chemistry - A European Journal, 2012, 18, 5676-5692.	1.7	131