

Rebecca Sure

List of Publications by Year in descending order

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Version: 2024-02-01

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	Corrected small basis set Hartree-Fock method for large systems. <i>Journal of Computational Chemistry</i> , 2013, 34, 1672-1685.	1.5	358
2	Comprehensive Benchmark of Association (Free) Energies of Realistic Host-Guest Complexes. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3785-3801.	2.3	188
3	Borylene Complexes (BH) ₂ and Nitrogen Cation Complexes (N ⁺) ₂ : Isoelectronic Homologues of Carbones CL ₂ . <i>Chemistry - A European Journal</i> , 2012, 18, 5676-5692.	1.7	131
4	Using dispersion-corrected density functional theory to understand supramolecular binding thermodynamics. <i>Chemical Communications</i> , 2015, 51, 1764-1774.	2.2	125
5	Substituent Effects and Supramolecular Interactions of Titanocene(III) Chloride: Implications for Catalysis in Single Electron Steps. <i>Journal of the American Chemical Society</i> , 2014, 136, 1663-1671.	6.6	78
6	Blind Prediction of Binding Affinities for Charged Supramolecular Host-Guest Systems: Achievements and Shortcomings of DFT-D3. <i>Journal of Physical Chemistry B</i> , 2014, 118, 3431-3440.	1.2	77
7	Mechanistic Study of the Titanocene(III)-Catalyzed Radical Arylation of Epoxides. <i>Chemistry - A European Journal</i> , 2015, 21, 280-289.	1.7	71
8	HYDROPHOBE Challenge: A Joint Experimental and Computational Study on the Host-Guest Binding of Hydrocarbons to Cucurbiturils, Allowing Explicit Evaluation of Guest Hydration Free-Energy Contributions. <i>Journal of Physical Chemistry B</i> , 2017, 121, 11144-11162.	1.2	62
9	Comprehensive theoretical study of all 1812 C ₆₀ isomers. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 14296-14305.	1.3	58
10	Small Atomic Orbital Basis Set First-Principles Quantum Chemical Methods for Large Molecular and Periodic Systems: A Critical Analysis of Error Sources. <i>ChemistryOpen</i> , 2016, 5, 94-109.	0.9	57
11	Highly Active Titanocene Catalysts for Epoxide Hydrosilylation: Synthesis, Theory, Kinetics, EPR Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 7671-7675.	7.2	57
12	Bismuth as a versatile cation for luminescence in coordination polymers from BiX ₃ /4,4'-bipy: understanding of photophysics by quantum chemical calculations and structural parallels to lanthanides. <i>Dalton Transactions</i> , 2018, 47, 7669-7681.	1.6	43
13	Synthesis, Chiral Resolution, and Absolute Configuration of Dissymmetric 4,15-Difunctionalized [2.2]Paracyclophanes. <i>Journal of Organic Chemistry</i> , 2014, 79, 6679-6687.	1.7	33
14	A systematic study of rare gas atoms encapsulated in small fullerenes using dispersion corrected density functional theory. <i>Journal of Computational Chemistry</i> , 2015, 36, 88-96.	1.5	28
15	Computational study of the rate constants and free energies of intramolecular radical addition to substituted anilines. <i>Beilstein Journal of Organic Chemistry</i> , 2013, 9, 1620-1629.	1.3	27
16	Hochaktive Titanocen-Katalysatoren für Epoxid-Hydrosilylierungen – Synthese, Theorie, Kinetik, EPR-Spektroskopie. <i>Angewandte Chemie</i> , 2016, 128, 7801-7805.	1.6	27
17	Halogen bonded supramolecular capsules: a challenging test case for quantum chemical methods. <i>Chemical Communications</i> , 2016, 52, 9893-9896.	2.2	26
18	Nearly Degenerate Isomers of C(BH) ₂ : Cumulene, Carbene, or Carbone?. <i>Chemistry - A European Journal</i> , 2013, 19, 15941-15954.	1.7	25

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19	Towards a converged strategy for including microsolvation in reaction mechanism calculations. Journal of Computer-Aided Molecular Design, 2021, 35, 473-492.	1.3	23
20	Quantum Chemical Dissection of the Shortest P=O...â€¦â€¦I Halogen Bond: The Decisive Role of Crystal Packing Effects. Chemistry - A European Journal, 2017, 23, 5687-5691.	1.7	20
21	From small fullerenes to the graphene limit: A harmonic forceâ€¦field method for fullerenes and a comparison to density functional calculations for <sc>C</sc>oldbergâ€¦<sc>C</sc>oxeter fullerenes up to C₉₈₀. Journal of Computational Chemistry, 2016, 37, 10-17.	1.5	12