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List of Publications by Year
in descending order

22 papers	191 citations	1163117 8 h-index	1125743 13 g-index
23 all docs	23 docs citations	23 times ranked	212 citing authors

#	Article	IF	Citations
1	Lithium complexes of doped phosphorene nanoflakes with aluminum, silicon and sulfur. Computational and Theoretical Chemistry, 2022, 1209, 113599.	2.5	3
2	Synthesis and characterization of organotin(IV) semiconductors and their applications in optoelectronics. Journal of Physics and Chemistry of Solids, 2021, 150, 109840.	4.0	6
3	Water clusters as bifunctional catalysts in organic chemistry: the hydrolysis of oxirane and its methyl derivatives. Organic and Biomolecular Chemistry, 2021, 19, 6776-6780.	2.8	9
4	Bifunctional squaramides with benzyl-like fragments: analysis of CHâ‹¯Ï€ interactions by a multivariate linear regression model and quantum chemical topology. Organic Chemistry Frontiers, 2021, 8, 3217-3227.	4.5	5
5	Novel 2D allotropic forms and nanoflakes of silicon, phosphorus, and germanium: a computational study. Journal of Molecular Modeling, 2021, 27, 142.	1.8	5
6	In silico modeling: electronic properties of phosphorene monoflakes and biflakes substituted with Al, Si, and S heteroatoms. Journal of Molecular Modeling, 2021, 27, 171.	1.8	3
7	Oligomeric approach to 2D materials modeling. Mundo Nano Revista Interdisciplinaria En Nanociencia Y NanotecnologÃa, 2021, 15, 1e-19e.	0.1	0
8	The electronic structure of van der Waals heterostructures formed by the nanoflakes of black phosphorene with those of graphene and haeckelites: their complexes with Li. Journal of Molecular Modeling, 2020, 26, 204.	1.8	2
9	On the strength of hydrogen bonding within water clusters on the coordination limit. Journal of Computational Chemistry, 2020, 41, 2266-2277.	3.3	20
10	Synthesis and photophysical properties of conformationally restricted difluoroboron Î²-diketonate complexes of 1-indanone derivatives. Tetrahedron, 2020, 76, 131457.	1.9	2
11	Electronic structure of hybrid pentaheptite carbon nanoflakes containing boron-nitrogen motifs. Journal of Molecular Modeling, 2020, 26, 72.	1.8	2
12	Stability of doubly and triply H-bonded complexes governed by acidityâ€“basicity relationships. Chemical Communications, 2019, 55, 1556-1559.	4.1	13
13	The effect of chiral N-substituents with methyl or trifluoromethyl groups on the catalytic performance of mono- and bifunctional thioureas. Organic and Biomolecular Chemistry, 2019, 17, 10045-10051.	2.8	8
14	Acidity and basicity interplay in amide and imide self-association. Chemical Science, 2018, 9, 4402-4413.	7.4	28
15	Simple method to estimate relative hydrogen bond basicities of amides and imides in chloroform. Journal of Molecular Structure, 2018, 1173, 608-611.	3.6	4
16	The bifunctional catalytic role of water clusters in the formation of acid rain. Chemical Communications, 2017, 53, 3516-3519.	4.1	24
17	Design and application of a bifunctional organocatalyst guided by electron density topological analyses. Catalysis Science and Technology, 2017, 7, 4470-4477.	4.1	10
18	Bifunctional Thioureas with Î±-Trifluoromethyl or Methyl Groups: Comparison of Catalytic Performance in Michael Additions. Journal of Organic Chemistry, 2016, 81, 7419-7431.	3.2	25

#	Article	IF	Citations
19	Electronic Structure and Noncovalent Interactions within Ionâ€“Radical Complexes of N-(2-Furylmethyl)aniline Molecular Ions. Journal of Physical Chemistry A, 2015, 119, 2098-2110.	2.5	4
20	Relationships between DFT/RRKM Branching Ratios of the Complementary Fragment Ions [C5H5O]+ and [M â€“ C5H5O]+ and Relative Abundances in the EI Mass Spectrum of N-(2-Furylmethyl)aniline. Journal of Physical Chemistry A, 2012, 116, 12136-12147.	2.5	5
21	Density functional theory and RRKM calculations of decompositions of the metastable Eâ€2,4â€pentadienal molecular ions. Journal of Mass Spectrometry, 2010, 45, 722-733.	1.6	5
22	Density functional theory and RRKM calculations of the gasâ€phase unimolecular rearrangements of methylfuran and pyran ions before fragmentations. Journal of Mass Spectrometry, 2009, 44, 1452-1458.	1.6	8