Manoj Kumar Kesharwani

List of Publications by Year
in descending order

50 papers	2,811 citations	377584 21 h-index	214428 50 g-index
50 all docs	50 docs citations	50 times ranked	4038 citing authors

#	Article	IF	Citations
1	New copper(II) complexes with (Z)-Nâ€²-{(2-hydroxynaphthalen-1-yl}methylene)acetohydrazide]: X-ray structure, Hirshfeld analysis, X-band electron paramagnetic resonance spectra, TD-DFT calculations and superoxide dismutase mimetic activity. Polyhedron, 2021, 195, 114969.	1.0	10
2	Charge Distribution in Cationic Molybdenum Imido Alkylidene N-Heterocyclic Carbene Complexes: A Combined X-ray, XAS, XES, DFT, MÃ¶ssbauer, and Catalysis Approach. ACS Catalysis, 2020, 10, 14810-14823.	5.5	19
3	Reaction Mechanism of Ring-Closing Metathesis with a Cationic Molybdenum Imido Alkylidene N-Heterocyclic Carbene Catalyst. Organometallics, 2020, 39, 3146-3159.	1.1	2
4	The X40Ã—10 Halogen Bonding Benchmark Revisited: Surprising Importance of (nâ€“1)d Subvalence Correlation. Journal of Physical Chemistry A, 2018, 122, 2184-2197.	1.1	34
5	Do CCSD and approximate CCSD-F12 variants converge to the same basis set limits? The case of atomization energies. Journal of Chemical Physics, 2018, 149, 154109.	1.2	48
6	The S66 Non-Covalent Interactions Benchmark Reconsidered Using Explicitly Correlated Methods Near the Basis Set Limit. Australian Journal of Chemistry, 2018, 71, 238.	0.5	40
7	Chirality-induced spin polarization places symmetry constraints on biomolecular interactions. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2474-2478.	3.3	155
8	Conventional and Explicitly Correlated ab Initio Benchmark Study on Water Clusters: Revision of the BEGDB and WATER27 Data Sets. Journal of Chemical Theory and Computation, 2017, 13, 3136-3152.	2.3	81
9	The aug-cc-pVnZ-F12 basis set family: Correlation consistent basis sets for explicitly correlated benchmark calculations on anions and noncovalent complexes. Journal of Chemical Physics, 2017, 147, 134106.	1.2	50
10	Surprising performance for vibrational frequencies of the distinguishable clusters with singles and doubles (DCSD) and MP2.5 approximations. AIP Conference Proceedings, 2017, , .	0.3	9
11	MP2-F12 basis set convergence for the S66 noncovalent interactions benchmark: Transferability of the complementary auxiliary basis set (CABS). AIP Conference Proceedings, 2017, , .	0.3	4
12	The S66x8 benchmark for noncovalent interactions revisited: explicitly correlated ab initio methods and density functional theory. Physical Chemistry Chemical Physics, 2016, 18, 20905-20925.	1.3	182
13	Benchmark ab Initio Conformational Energies for the Proteinogenic Amino Acids through Explicitly Correlated Methods. Assessment of Density Functional Methods. Journal of Chemical Theory and Computation, 2016, 12, 444-454.	2.3	99
14	Comment on â€œDoubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0â€•[J. Chem. Phys. 136, 174103 (2012)]. Journal of Chemical Physics, 2015, 143, 187101.	1.2	13
15	In silico study on aging and reactivation processes of tabun conjugated AChE. MedChemComm, 2015, 6, 871-878.	3.5	6
16	Exploring the Accuracy Limits of Local Pair Natural Orbital Coupled-Cluster Theory. Journal of Chemical Theory and Computation, 2015, 11, 1525-1539.	2.3	544
17	The cc-pV5Z-F12 basis set: reaching the basis set limit in explicitly correlated calculations. Molecular Physics, 2015, 113, 1551-1558.	0.8	57
18	Frequency and Zero-Point Vibrational Energy Scale Factors for Double-Hybrid Density Functionals (and Other Selected Methods): Can Anharmonic Force Fields Be Avoided?. Journal of Physical Chemistry A, 2015, 119, 1701-1714.	1.1	441

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19	Explicitly correlated coupled cluster benchmarks with realistic-sized ligands for some late-transition metal reactions: basis sets convergence and performance of more approximate methods. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	37
20	Some Observations on Counterpoise Corrections for Explicitly Correlated Calculations on Noncovalent Interactions. Journal of Chemical Theory and Computation, 2014, 10, 3791-3799.	2.3	109
21	Assessment of CCSD(T)-F12 Approximations and Basis Sets for Harmonic Vibrational Frequencies. Journal of Chemical Theory and Computation, 2014, 10, 2085-2090.	2.3	61
22	Dipicrylamine as a colorimetric sensor for anions: experimental and computational study. RSC Advances, 2014, 4, 53273-53281.	1.7	10
23	Origin of reversal of stereoselectivity for [4+2] cycloaddition reaction between cyclopentadiene and methyl methacrylate in the presence of the chloroloaluminate ionic liquid (1-ethyl-3-methyl-imidazolium chloride): in silico studies. Canadian Journal of Chemistry, 2014, 92, 862-867.	0.6	2
24	Hydrogen Bonding Interaction between Active Methylene Hydrogen Atoms and an Anion as a Binding Motif for Anion Recognition: Experimental Studies and Theoretical Rationalization. Journal of Physical Chemistry A, 2014, 118, 2656-2666.	1.1	9
25	Heats of formation of the amino acids re-examined by means of W1-F12 and W2-F12 theories. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	74
26	Molecular Interactions, Proton Exchange, and Photoinduced Processes Prompted by an Inclusion Process and a [2]Pseudorotaxane Formation. Journal of Organic Chemistry, 2013, 78, 9004-9012.	1.7	11
27	Conformational preference of glycinamide in solution: An answer derived from combined experimental and computational studies. Journal of Molecular Graphics and Modelling, 2013, 46, 52-58.	1.3	1
28	In silico studies toward the recognition of fluoride ion by novel bicyclic diborane receptors and tuning through remote substituent effects. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	2
29	In Silico Studies in Probing the Role of Kinetic and Structural Effects of Different Drugs for the Reactivation of Tabun-Inhibited AChE. PLoS ONE, 2013, 8, e79591.	1.1	10
30	Ratiometric Detection of Cr³⁺ and Hg²⁺ by a Naphthalimide-Rhodamine Based Fluorescent Probe. Inorganic Chemistry, 2012, 51, 1769-1777.	1.9	306
31	An alternative approach: a highly selective dual responding fluoride sensor having active methylene group as binding site. Organic and Biomolecular Chemistry, 2012, 10, 2263.	1.5	20
32	Rational design of a new class of polycyclic organic bases bearing two superbasic sites and their applications in the CO2 capture and activation process. Chemical Communications, 2012, 48, 5865.	2.2	28
33	In silico studies toward the recognition of fluoride ion by substituted borazines. Journal of Molecular Graphics and Modelling, 2012, 38, 363-368.	1.3	1
34	Probing O-dealkylation and deamination aging processes in tabun-conjugated AChE: a computational study. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	2
35	Folding and Unfolding Movements in a [2]Pseudorotaxane. Journal of Organic Chemistry, 2011, 76, 138-144.	1.7	39
36	Receptor design and extraction of inorganic fluoride ion from aqueous medium. Chemical Communications, 2011, 47, 7398.	2.2	49

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37	Hydrolysis and retroâ€aldol cleavage of ethyl threoâ€2â€(1â€adamantyl)â€3â€hydroxybutyrate: competing reactions. Journal of Physical Organic Chemistry, 2011, 24, 578-587.	0.9	5
38	Zn^{II}â€“2,2â€²:6â€²,2â€³â€Terpyridineâ€Based Complex as Fluorescent Chemosensor for PPi, AMP and ADP. European Journal of Inorganic Chemistry, 2011, 2011, 3050-3058.	1.0	63
39	Probing the structural and electronic effects to stabilize nonplanar forms of thioamide derivatives: A computational study. Journal of Computational Chemistry, 2011, 32, 2170-2176.	1.5	10
40	Borazine as a sensor for fluoride ion: a computational and experimental study. Tetrahedron Letters, 2011, 52, 3636-3639.	0.7	17
41	Solvolysis process of organophosphorus compound P-[2-(dimethylamino)ethyl]-N,N-dimethylphosphonamidic fluoride with simple and Î±-nucleophiles: a DFT study. Theoretical Chemistry Accounts, 2010, 127, 39-47.	0.5	13
42	Anion recognition through hydrogen bonding by adamantane-dipyrromethane receptors. Tetrahedron, 2010, 66, 1689-1698.	1.0	17
43	Remarkable effect of hydroxylamine anion towards the solvolysis of sarin: A DFT study. Computational and Theoretical Chemistry, 2010, 944, 132-136.	1.5	13
44	Differential binding of bispyridinium oxime drugs with acetylcholinesterase. Acta Pharmacologica Sinica, 2010, 31, 313-328.	2.8	18
45	An Experimental and Theoretical Study on the Remarkable Influence of Protecting Groups on the Selectivity of Addition of Amines to Vinyl Sulfone-Modified Hex-2-enopyranosides. Journal of Organic Chemistry, 2010, 75, 303-314.	1.7	10
46	Probing the Influence of Anomeric Effects on the Lithium Ion Affinity in 1,3-Diaza Systems: A Computational Study. Journal of Physical Chemistry A, 2010, 114, 10684-10693.	1.1	8
47	Influence of Formamide on the Crystal Habit of LiF, NaCl, and KI: A DFT and Aqueous Solvent Model Study. Crystal Growth and Design, 2009, 9, 77-81.	1.4	24
48	Solvolysis of chemical warfare agent VX is more efficient with hydroxylamine anion: A computational study. Journal of Molecular Graphics and Modelling, 2009, 28, 177-182.	1.3	20
49	Syntheses, structures and electrochemical properties of complexes of nickel(II) with triethylenetetramine and bidentate nitrogen donor co-ligands. Transition Metal Chemistry, 2008, 33, 733-738.	0.7	19
50	Synthetic and Theoretical Investigations on the Construction of Oxanorbornenes by a Michael Addition and Intramolecular Dielsâ€“Alder Furan Reaction. European Journal of Organic Chemistry, 2008, 2008, 6106-6118.	1.2	9