

# Saurabh Kumar Singh

## List of Publications by Year in descending order

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41  
papers

1,838  
citations

257357

24  
h-index

289141

40  
g-index

44  
all docs

44  
docs citations

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times ranked

1725  
citing authors

#	ARTICLE	IF	CITATIONS
1	Neosilyllithium-Catalyzed Hydroboration of Alkynes and Alkenes in the Presence of Pinacolborane (HBpin). <i>European Journal of Inorganic Chemistry</i> , 2022, 2022, .	1.0	5
2	Solvent mediated synthesis of homoleptic tri and tetranuclear nickel complex derived from $[\text{Ni}_2(\mu\text{-SeC}_5\text{H}_4\text{N})_2(\text{dppe})_2]^{2+}$ and theoretical studies. <i>Journal of Organometallic Chemistry</i> , 2022, 957, 122177.	0.8	2
3	Tuning the structure and magnetic properties <i>via</i> distinct pyridine derivatives in cobalt(II) coordination polymers. <i>Dalton Transactions</i> , 2022, 51, 695-704.	1.6	20
4	Zero-field Slow Magnetic Relaxation Behavior of $\text{Dy}_2$ in a Series of Dinuclear $\{\text{Ln}_2\}$ ( $\text{Ln}=\text{Dy}, \text{Tb}, \text{Gd}$ and $\text{Er}$ ) Complexes: A Combined Experimental and Theoretical Study. <i>European Journal of Inorganic Chemistry</i> , 2022, 2022, .	1.0	9
5	A $\text{Nd}_6$ molecular butterfly: a unique all-in-one material for SMM, MCE and maiden photosensitized opto-electronic device fabrication. <i>Dalton Transactions</i> , 2022, 51, 1617-1633.	1.6	7
6	Unsaturated Sulfur Crown Ethers Can Extract Mercury(II) and Show Promise for Future Copernicium(II) Studies: A Combined Experimental and Computational Study. <i>Inorganic Chemistry</i> , 2022, 61, 807-817.	1.9	1
7	Tuning chain topologies and magnetic anisotropy in one-dimensional cobalt(II) coordination polymers <i>via</i> distinct dicarboxylates. <i>CrystEngComm</i> , 2022, 24, 3928-3937.	1.3	11
8	Synthesis of $[(\text{CO})_5\text{MS}=\text{CFcCH}_3]$ and exploration of the nature of M-S vs. M-O bonds in $[(\text{CO})_5\text{ME}=\text{CFcCH}_3]$ ; ( $\text{M}=\text{Cr}, \text{Mo}, \text{W}$ and $\text{E}=\text{O}, \text{S}$ ) complexes. <i>Journal of Organometallic Chemistry</i> , 2021, 954-955, 122080.	0.8	0
9	A serendipitous isolation of cocrystallized platinum-tin complexes: synthesis, structure and theoretical exploration. <i>New Journal of Chemistry</i> , 2020, 44, 20945-20955.	1.4	1
10	Slow magnetic relaxation in a homo dinuclear $\text{Dy}_2$ complex in a pentagonal bipyramidal geometry. <i>Dalton Transactions</i> , 2020, 49, 13110-13122.	1.6	16
11	Correlating Electronic Structure and Magnetic Anisotropy in Actinide Complexes $[\text{An}(\text{COT})_2]$ , $\text{An}^{\text{III/IV}} = \text{U}, \text{Np},$ and $\text{Pu}$ . <i>Inorganic Chemistry</i> , 2020, 59, 6815-6825.	1.9	21
12	Role of (1,3) {Cu-Cu} Interaction on the Magneto-Caloric Effect of Trinuclear $\{\text{Cu}^{\text{II}}\text{-Gd}^{\text{III}}\text{-Cu}^{\text{II}}\}$ Complexes: Combined DFT and Experimental Studies. <i>Inorganic Chemistry</i> , 2018, 57, 1846-1858.	1.9	34
13	Challenges in Multireference Perturbation Theory for the Calculations of the <i>g</i> -Tensor of First-Row Transition-Metal Complexes. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4662-4677.	2.3	55
14	Role of the Diamagnetic Zinc(II) Ion in Determining the Electronic Structure of Lanthanide Single-Ion Magnets. <i>Chemistry - A European Journal</i> , 2017, 23, 4903-4916.	1.7	72
15	Role of Halide Ions in the Nature of the Magnetic Anisotropy in Tetrahedral Co II Complexes. <i>Chemistry - A European Journal</i> , 2017, 23, 9546-9559.	1.7	48
16	Covalency and chemical bonding in transition metal complexes: An ab initio based ligand field perspective. <i>Coordination Chemistry Reviews</i> , 2017, 344, 2-25.	9.5	178
17	Influence of the Ligand Field on the Slow Relaxation of Magnetization of Unsymmetrical Monomeric Lanthanide Complexes: Synthesis and Theoretical Studies. <i>Inorganic Chemistry</i> , 2017, 56, 14260-14276.	1.9	33
18	Key role of higher order symmetry and electrostatic ligand field design in the magnetic relaxation of low-coordinate $\text{Er}_2$ complexes. <i>Dalton Transactions</i> , 2017, 46, 11913-11924.	1.6	23

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19	[Os <sub>6</sub> ] <sup>x</sup> : Molecular Models for Spin-Orbit Entangled Phenomena. Chemistry - A European Journal, 2017, 23, 11244-11248.	1.7	18
20	Role of Magnetic Exchange Interactions in the Magnetization Relaxation of {3d <sup>4f</sup> } Single-Molecule Magnets: A Theoretical Perspective. Chemistry - A European Journal, 2016, 22, 672-680.	1.7	55
21	Theoretical insights into the origin of magnetic exchange and magnetic anisotropy in {Re <sup>IV</sup> â€M <sup>II</sup> } (M = Mn, Fe, Co, Ni and Cu) single chain magnets. Dalton Transactions, 2016, 45, 8201-8214.	1.6	12
22	What Controls the Sign and Magnitude of Magnetic Anisotropy in Tetrahedral Cobalt(II) Single-Ion Magnets?. Inorganic Chemistry, 2016, 55, 9564-9578.	1.9	100
23	Observation of Slow Relaxation and Single-Molecule Toroidal Behavior in a Family of Butterfly-Shaped Ln <sub>4</sub> Complexes. Chemistry - A European Journal, 2016, 22, 18532-18550.	1.7	39
24	Deciphering the origin of giant magnetic anisotropy and fast quantum tunnelling in Rhenium(IV) single-molecule magnets. Nature Communications, 2016, 7, 10669.	5.8	32
25	Magnetic Relaxation in Single-Electron Single-Ion Cerium(III) Magnets: Insights from Ab Initio Calculations. Chemistry - A European Journal, 2015, 21, 13812-13819.	1.7	56
26	Origin of SMM behaviour in an asymmetric Er( <sup>iii</sup> ) Schiff base complex: a combined experimental and theoretical study. Chemical Communications, 2015, 51, 6137-6140.	2.2	53
27	A synthetic strategy for switching the single ion anisotropy in tetrahedral Co( <sup>ii</sup> ) complexes. Chemical Communications, 2015, 51, 3739-3742.	2.2	113
28	Magnetic Anisotropy of Mononuclear Ni <sup>II</sup> Complexes: On the Importance of Structural Diversity and the Structural Distortions. Chemistry - A European Journal, 2014, 20, 10305-10313.	1.7	50
29	Can Anisotropic Exchange Be Reliably Calculated Using Density Functional Methods? A Case Study on Trinuclear Mn <sup>III</sup> â€M <sup>III</sup> â€Mn <sup>III</sup> (M=Fe, Ru, and Os) Cyanometalate Single-Molecule Magnets. Chemistry - A European Journal, 2014, 20, 113-123.	1.7	20
30	Unprecedented magnetic relaxation via the fourth excited state in low-coordinate lanthanide single-ion magnets: a theoretical perspective. Chemical Communications, 2014, 50, 15513-15516.	2.2	65
31	Magnetic Anisotropy and Mechanism of Magnetic Relaxation in Er(III) Single-Ion Magnets. Inorganic Chemistry, 2014, 53, 10835-10845.	1.9	86
32	Probing the Origin of Magnetic Anisotropy in a Dinuclear {Mn <sup>III</sup> Cu <sup>II</sup> } Single-Molecule Magnet: The Role of Exchange Anisotropy. Chemistry - A European Journal, 2014, 20, 5214-5218.	1.7	36
33	Enhancing the effective energy barrier of a Dy( <sup>iii</sup> ) SMM using a bridged diamagnetic Zn( <sup>ii</sup> ) ion. Chemical Communications, 2014, 50, 8838-8841.	2.2	134
34	Fluoride-Bridged {Gd <sup>III</sup> <sub>3</sub> M <sup>III</sup> <sub>2</sub> } (M=Cr, Fe, Ga) Molecular Magnetic Refrigerants. Angewandte Chemie - International Edition, 2014, 53, 2394-2397.	7.2	86
35	Enhancing the double exchange interaction in a mixed valence {VIIIâ€VII} pair: a theoretical perspective. Dalton Transactions, 2013, 42, 16490.	1.6	18
36	Angular dependence of the exchange interaction in fluoride-bridged Gd <sup>III</sup> â€Cr <sup>III</sup> complexes. Chemical Communications, 2013, 49, 5583.	2.2	33

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37	Decisive interactions that determine ferro/antiferromagnetic coupling in {3d <sup>4</sup> } pairs: a case study on dinuclear {V(IV)–Gd(III)} complexes. Dalton Transactions, 2013, 42, 3623.	1.6	51
38	Synthetic, structural, spectroscopic and theoretical study of a Mn(III)–Cu(II) dimer containing a Jahn–Teller compressed Mn ion. Dalton Transactions, 2013, 42, 207-216.	1.6	16
39	A computational perspective on magnetic coupling, magneto-structural correlations and magneto-caloric effect of a ferromagnetically coupled {Gd(III)–Gd(III)} Pair. Polyhedron, 2013, 52, 1299-1305.	1.0	53
40	Theoretical studies on {3d-Gd} and {3d-Gd-3d} complexes: Effect of metal substitution on the effective exchange interaction. Polyhedron, 2013, 66, 81-86.	1.0	30
41	Density functional studies on dinuclear {Ni(II)Gd(III)} and trinuclear {Ni(II)Gd(III)Ni(II)} complexes: magnetic exchange and magneto-structural maps. Dalton Transactions, 2011, 40, 10897.	1.6	132