

# Saurabh Kumar Singh

## List of Publications by Year in descending order

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Version: 2024-02-01

41  
papers

1,838  
citations

257357

24  
h-index

289141

40  
g-index

44  
all docs

44  
docs citations

44  
times ranked

1725  
citing authors

#	ARTICLE	IF	CITATIONS
1	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
2	Enhancing the effective energy barrier of a Dy( $\text{III}$ ) SMM using a bridged diamagnetic Zn( $\text{II}$ ) ion. <i>Chemical Communications</i> , 2014, 50, 8838-8841.	2.2	134
3	Density functional studies on dinuclear $\{\text{NiII} \text{GdIII}\}$ and trinuclear $\{\text{NiII} \text{GdIII} \text{NiII}\}$ complexes: magnetic exchange and magneto-structural maps. <i>Dalton Transactions</i> , 2011, 40, 10897.	1.6	132
4	A synthetic strategy for switching the single ion anisotropy in tetrahedral Co( $\text{II}$ ) complexes. <i>Chemical Communications</i> , 2015, 51, 3739-3742.	2.2	113
5	What Controls the Sign and Magnitude of Magnetic Anisotropy in Tetrahedral Cobalt(II) Single-Ion Magnets?. <i>Inorganic Chemistry</i> , 2016, 55, 9564-9578.	1.9	100
6	Magnetic Anisotropy and Mechanism of Magnetic Relaxation in Er(III) Single-Ion Magnets. <i>Inorganic Chemistry</i> , 2014, 53, 10835-10845.	1.9	86
7	Fluoride-Bridged $\{\text{Gd}^{\text{III}}\}_3\text{M}^{\text{II}}_2$ ( $\text{M}=\text{Cr}, \text{Fe}, \text{Ga}$ ) Molecular Magnetic Refrigerants. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 2394-2397.	7.2	86
8	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
9	Unprecedented magnetic relaxation via the fourth excited state in low-coordinate lanthanide single-ion magnets: a theoretical perspective. <i>Chemical Communications</i> , 2014, 50, 15513-15516.	2.2	65
10	Magnetic Relaxation in Single-Electron Single-Ion Cerium(III) Magnets: Insights from Ab Initio Calculations. <i>Chemistry - A European Journal</i> , 2015, 21, 13812-13819.	1.7	56
11	Role of Magnetic Exchange Interactions in the Magnetization Relaxation of $\{3d^4\}$ Single-Molecule Magnets: A Theoretical Perspective. <i>Chemistry - A European Journal</i> , 2016, 22, 672-680.	1.7	55
12	Challenges in Multireference Perturbation Theory for the Calculations of the $\langle i   g   i \rangle$ -Tensor of First-Row Transition-Metal Complexes. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4662-4677.	2.3	55
13	A computational perspective on magnetic coupling, magneto-structural correlations and magneto-caloric effect of a ferromagnetically coupled $\{\text{GdIII} \text{GdIII}\}$ Pair. <i>Polyhedron</i> , 2013, 52, 1299-1305.	1.0	53
14	Origin of SMM behaviour in an asymmetric Er( $\text{III}$ ) Schiff base complex: a combined experimental and theoretical study. <i>Chemical Communications</i> , 2015, 51, 6137-6140.	2.2	53
15	Decisive interactions that determine ferro/antiferromagnetic coupling in $\{3d^4\}$ pairs: a case study on dinuclear $\{\text{V(IV)} \text{Gd(III)}\}$ complexes. <i>Dalton Transactions</i> , 2013, 42, 3623.	1.6	51
16	Magnetic Anisotropy of Mononuclear Ni( $\text{II}$ ) Complexes: On the Importance of Structural Diversity and the Structural Distortions. <i>Chemistry - A European Journal</i> , 2014, 20, 10305-10313.	1.7	50
17	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
18	Observation of Slow Relaxation and Single-Molecule Toroidal Behavior in a Family of Butterfly-Shaped $\text{Ln}_{\text{4}}$ Complexes. <i>Chemistry - A European Journal</i> , 2016, 22, 18532-18550.	1.7	39

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19	Probing the Origin of Magnetic Anisotropy in a Dinuclear $\{Mn^{III}Cu^{II}\}$ Single-Molecule Magnet: The Role of Exchange Anisotropy. <i>Chemistry - A European Journal</i> , 2014, 20, 5214-5218.	1.7	36
20	Role of (1,3) $\{Cu-Cu\}$ Interaction on the Magneto-Caloric Effect of Trinuclear $\{Cu^{II}-Gd^{III}-Cu^{II}\}$ Complexes: Combined DFT and Experimental Studies. <i>Inorganic Chemistry</i> , 2018, 57, 1846-1858.	1.9	34
21	Angular dependence of the exchange interaction in fluoride-bridged $Gd^{III}-Cr^{III}$ complexes. <i>Chemical Communications</i> , 2013, 49, 5583.	2.2	33
22	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
23	Deciphering the origin of giant magnetic anisotropy and fast quantum tunnelling in Rhenium(IV) single-molecule magnets. <i>Nature Communications</i> , 2016, 7, 10669.	5.8	32
24	Theoretical studies on $\{3d-Gd\}$ and $\{3d-Gd-3d\}$ complexes: Effect of metal substitution on the effective exchange interaction. <i>Polyhedron</i> , 2013, 66, 81-86.	1.0	30
25	Key role of higher order symmetry and electrostatic ligand field design in the magnetic relaxation of low-coordinate $Er^{III}$ complexes. <i>Dalton Transactions</i> , 2017, 46, 11913-11924.	1.6	23
26	Correlating Electronic Structure and Magnetic Anisotropy in Actinide Complexes $[An(COT)_2]$ , $An^{III/IV}$ = U, Np, and Pu. <i>Inorganic Chemistry</i> , 2020, 59, 6815-6825.	1.9	21
27	Can Anisotropic Exchange Be Reliably Calculated Using Density Functional Methods? A Case Study on Trinuclear $Mn^{III}-M^{III}-Mn^{III}$ ( $M=Fe, Ru, \text{ and } Os$ ) Cyanometalate Single-Molecule Magnets. <i>Chemistry - A European Journal</i> , 2014, 20, 113-123.	1.7	20
28	Tuning the structure and magnetic properties <i>via</i> distinct pyridine derivatives in cobalt( $Co^{II}$ ) coordination polymers. <i>Dalton Transactions</i> , 2022, 51, 695-704.	1.6	20
29	Enhancing the double exchange interaction in a mixed valence $\{VIII-VII\}$ pair: a theoretical perspective. <i>Dalton Transactions</i> , 2013, 42, 16490.	1.6	18
30	$[Os_6]^{x+}$ : Molecular Models for Spin-Orbit Entangled Phenomena. <i>Chemistry - A European Journal</i> , 2017, 23, 11244-11248.	1.7	18
31	Synthetic, structural, spectroscopic and theoretical study of a $Mn^{III}-Cu^{II}$ dimer containing a Jahn-Teller compressed Mn ion. <i>Dalton Transactions</i> , 2013, 42, 207-216.	1.6	16
32	Slow magnetic relaxation in a homo dinuclear $Dy^{III}$ complex in a pentagonal bipyramidal geometry. <i>Dalton Transactions</i> , 2020, 49, 13110-13122.	1.6	16
33	Theoretical insights into the origin of magnetic exchange and magnetic anisotropy in $\{Re^{IV}-M^{II}\}$ ( $M = Mn, Fe, Co, Ni \text{ and } Cu$ ) single chain magnets. <i>Dalton Transactions</i> , 2016, 45, 8201-8214.	1.6	12
34	Tuning chain topologies and magnetic anisotropy in one-dimensional cobalt( $Co^{II}$ ) coordination polymers <i>via</i> distinct dicarboxylates. <i>CrystEngComm</i> , 2022, 24, 3928-3937.	1.3	11
35	Zero-field Slow Magnetic Relaxation Behavior of $Dy_2$ in a Series of Dinuclear $\{Ln_2\}$ ( $Ln=Dy, Tb, Gd \text{ and } Er$ ) Complexes: A Combined Experimental and Theoretical Study. <i>European Journal of Inorganic Chemistry</i> , 2022, 2022, .	1.0	9
36	A $Nd_6$ 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

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37	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
38	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
39	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
40	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
41	Synthesis of $[(\text{CO})_5\text{MS}=\text{CFcCH}_3]$ and exploration of the nature of M-S vs. M-O bonds in $[(\text{CO})_5\text{ME}=\text{CFcCH}_3]$ ; (M=Cr, Mo, W and E=O, S) complexes. <i>Journal of Organometallic Chemistry</i> , 2021, 954-955, 122080.	0.8	0