

Nathalie Guihã©ry

List of Publications by Year in descending order

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Version: 2024-02-01

20
papers

1,646
citations

516215

16
h-index

752256

20
g-index

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all docs

20
docs citations

20
times ranked

1609
citing authors

#	ARTICLE	IF	CITATIONS
1	Magnetic Interactions in Molecules and Highly Correlated Materials: Physical Content, Analytical Derivation, and Rigorous Extraction of Magnetic Hamiltonians. <i>Chemical Reviews</i> , 2014, 114, 429-492.	23.0	342
2	Universal Theoretical Approach to Extract Anisotropic Spin Hamiltonians. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2977-2984.	2.3	270
3	Origin of the Magnetic Anisotropy in Heptacoordinate Ni ^{II} and Co ^{II} Complexes. <i>Chemistry - A European Journal</i> , 2013, 19, 950-956.	1.7	145
4	Giant Ising-Type Magnetic Anisotropy in Trigonal Bipyramidal Ni(II) Complexes: Experiment and Theory. <i>Journal of the American Chemical Society</i> , 2013, 135, 3017-3026.	6.6	135
5	Direct generation of local orbitals for multireference treatment and subsequent uses for the calculation of the correlation energy. <i>Journal of Chemical Physics</i> , 2002, 116, 10060-10068.	1.2	107
6	Theoretical Determination of the Zero-Field Splitting in Copper Acetate Monohydrate. <i>Inorganic Chemistry</i> , 2011, 50, 6229-6236.	1.9	91
7	Rigorous Extraction of the Anisotropic Multispin Hamiltonian in Bimetallic Complexes from the Exact Electronic Hamiltonian. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 55-65.	2.3	76
8	Cyano-Bridged Fe(II)â€“Cr(III) Single-Chain Magnet Based on Pentagonal Bipyramid Units: On the Added Value of Aligned Axial Anisotropy. <i>Journal of the American Chemical Society</i> , 2018, 140, 7698-7704.	6.6	70
9	Pentagonal Bipyramid Fe ^{II} Complexes: Robust Isingâ€“Spin Units towards Heteropolynuclear Nanomagnets. <i>Chemistry - A European Journal</i> , 2017, 23, 4380-4396.	1.7	67
10	Pentanuclear Cyanide-Bridged Complexes Based on Highly Anisotropic Co ^{II} Seven-Coordinate Building Blocks: Synthesis, Structure, and Magnetic Behavior. <i>Inorganic Chemistry</i> , 2011, 50, 12045-12052.	1.9	66
11	Bond electron pair: Its relevance and analysis from the quantum chemistry point of view. <i>Journal of Computational Chemistry</i> , 2007, 28, 35-50.	1.5	64
12	Theoretical determination of spin Hamiltonians with isotropic and anisotropic magnetic interactions in transition metal and lanthanide complexes. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 18784.	1.3	45
13	Magnetic anisotropy in binuclear complexes in the weak-exchange limit: From the multispin to the giant-spin Hamiltonian. <i>Physical Review B</i> , 2010, 81, .	1.1	39
14	Interplay between Local Anisotropies in Binuclear Complexes. <i>Inorganic Chemistry</i> , 2014, 53, 4508-4516.	1.9	36
15	A Strategy to Determine Appropriate Active Orbitals and Accurate Magnetic Couplings in Organic Magnetic Systems. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4127-4137.	2.3	35
16	First-principles study of magnetic interactions in cupric oxide. <i>Physical Review B</i> , 2012, 85, .	1.1	26
17	How to create giant Dzyaloshinskiiâ€“Moriya interactions? Analytical derivation and <i>ab initio</i> calculations on model dicopper(II) complexes. <i>Journal of Chemical Physics</i> , 2021, 154, 134301.	1.2	10
18	Trinuclear Cyanidoâ€“Bridged [Cr ₂ Fe] Complexes: To Be or not to Be a Singleâ€“Molecule Magnet, a Matter of Straightness. <i>Chemistry - A European Journal</i> , 2021, 27, 15484-15495.	1.7	9

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19	Extraction of giant Dzyaloshinskiiâ€™Moriya interaction from <i>ab initio</i> calculations: First-order spinâ€™orbit coupling model and methodological study. <i>Journal of Chemical Physics</i> , 2021, 155, 164305.	1.2	8
20	Understanding the impact of correlation on bond length alternation in polyenes. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	5