RÃ©mi Maurice

List of Publications by Year
in descending order

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52	2,043	218381	233125
papers	citations	26 h-index	45 g-index

52	52	52	2293
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Universal Theoretical Approach to Extract Anisotropic Spin Hamiltonians. Journal of Chemical Theory and Computation, 2009, 5, 2977-2984.	2.3	270
2	Origin of the Magnetic Anisotropy in Heptacoordinate Ni^{II} and Co^{II} Complexes. Chemistry - A European Journal, 2013, 19, 950-956.	1.7	145
3	Giant Ising-Type Magnetic Anisotropy in Trigonal Bipyramidal Ni(II) Complexes: Experiment and Theory. Journal of the American Chemical Society, 2013, 135, 3017-3026.	6.6	135
4	Unusual structure, bonding and properties in a californium borate. Nature Chemistry, 2014, 6, 387-392.	6.6	110
5	Theoretical Determination of the Zero-Field Splitting in Copper Acetate Monohydrate. Inorganic Chemistry, 2011, 50, 6229-6236.	1.9	91
6	Role of the Metal in the Bonding and Properties of Bimetallic Complexes Involving Manganese, Iron, and Cobalt. Journal of the American Chemical Society, 2014, 136, 1842-1855.	6.6	91
7	Rigorous Extraction of the Anisotropic Multispin Hamiltonian in Bimetallic Complexes from the Exact Electronic Hamiltonian. Journal of Chemical Theory and Computation, 2010, 6, 55-65.	2.3	76
8	Pentanuclear Cyanide-Bridged Complexes Based on Highly Anisotropic Co^{II} Seven-Coordinate Building Blocks: Synthesis, Structure, and Magnetic Behavior. Inorganic Chemistry, 2011, 50, 12045-12052.	1.9	66
9	Experimental and computational evidence of halogen bonds involving astatine. Nature Chemistry, 2018, 10, 428-434.	6.6	63
10	Magnetic State of PyrochloreCd2Os2O7Emerging from Strong Competition of Ligand Distortions and Longer-Range Crystalline Anisotropy. Physical Review Letters, 2013, 110, 127206.	2.9	59
11	Magnetostructural relations from a combined ab initio and ligand field analysis for the nonintuitive zero-field splitting in Mn(III) complexes. Journal of Chemical Physics, 2010, 133, 084307.	1.2	54
12	Antisymmetric Magnetic Interactions in Oxo-Bridged Copper(II) Bimetallic Systems. Journal of Chemical Theory and Computation, 2010, 6, 3092-3101.	2.3	51
13	Advances on the Determination of the Astatine Pourbaix Diagram: Predomination of AtO(OH)₂^{â˜’} over At^{â˜’} in Basic Conditions. Chemistry - A European Journal, 2016, 22, 2964-2971.	1.7	46
14	Theoretical determination of spin Hamiltonians with isotropic and anisotropic magnetic interactions in transition metal and lanthanide complexes. Physical Chemistry Chemical Physics, 2013, 15, 18784.	1.3	45
15	CO₂ Adsorption in Fe₂(dobdc): A Classical Force Field Parameterized from Quantum Mechanical Calculations. Journal of Physical Chemistry C, 2014, 118, 12230-12240.	1.5	45
16	Targeted radionuclide therapy with astatine-211: Oxidative dehalogenation of astatobenzoate conjugates. Scientific Reports, 2017, 7, 2579.	1.6	45
17	Single-Ion Magnetic Anisotropy and Isotropic Magnetic Couplings in the Metalâ€“Organic Framework Fe₂(dobdc). Inorganic Chemistry, 2013, 52, 9379-9389.	1.9	43
18	Computational determination of the dominant triplet population mechanism in photoexcited benzophenone. Physical Chemistry Chemical Physics, 2014, 16, 25393-25403.	1.3	42

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19	Scrutinizing â€œInvisibleâ€•astatine: A challenge for modern density functionals. Journal of Computational Chemistry, 2016, 37, 1345-1354.	1.5	42
20	Magnetic anisotropy in binuclear complexes in the weak-exchange limit: From the multispin to the giant-spin Hamiltonian. Physical Review B, 2010, 81, .	1.1	39
21	Tools for Predicting the Nature and Magnitude of Magnetic Anisotropy in Transition Metal Complexes: Application to Co(II) Complexes. Magnetochemistry, 2016, 2, 31.	1.0	37
22	Interplay between Local Anisotropies in Binuclear Complexes. Inorganic Chemistry, 2014, 53, 4508-4516.	1.9	36
23	Magnetic Anisotropy in Ni^{II}â€“Y^{III} Binuclear Complexes: On the Importance of Both the First Coordination Sphere of the Ni^{II} Ion and the Y^{III} Ion Belonging to the Second Coordination Sphere. Inorganic Chemistry, 2011, 50, 11075-11081.	1.9	35
24	Pentacoordinate Ni^{II} Complexes: Preparation, Magnetic Measurements, and Ab Initio Calculations of the Magnetic Anisotropy Terms. Chemistry - A European Journal, 2012, 18, 4031-4040.	1.7	29
25	Effective bond orders from two-step spinâ€“orbit coupling approaches: The I2, At2, IO+, and AtO+ case studies. Journal of Chemical Physics, 2015, 142, 094305.	1.2	29
26	211 At-labeled agents for alpha-immunotherapy: On the inÂvivo stability of astatine-agent bonds. European Journal of Medicinal Chemistry, 2016, 116, 156-164.	2.6	28
27	First-principles study of magnetic interactions in cupric oxide. Physical Review B, 2012, 85, .	1.1	26
28	Magnetic interactions in LiCu2O2: Single-chain versus double-chain models. Physical Review B, 2012, 86, .	1.1	23
29	Synthesis and Structures of Plutonyl Nitrate Complexes: Is Plutonium Heptavalent in PuO₃(NO₃)₂^{â€“} ?. Inorganic Chemistry, 2015, 54, 2367-2373.	1.9	19
30	Identifying the Interactions That Allow Separation of O₂ from N₂ on the Open Iron Sites of Fe₂(dobdc). Journal of Physical Chemistry C, 2015, 119, 28499-28511.	1.5	18
31	Electronic structures and geometries of the XF3 (X = Cl, Br, I, At) fluorides. Journal of Chemical Physics, 2015, 143, 114306.	1.2	17
32	Thorium and Uranium Carbide Cluster Cations in the Gas Phase: Similarities and Differences between Thorium and Uranium. Inorganic Chemistry, 2013, 52, 10968-10975.	1.9	16
33	Adsorbate-Induced Changes in Magnetic Interactions in Fe₂(dobdc) with Adsorbed Hydrocarbon Molecules. Journal of Physical Chemistry C, 2016, 120, 9933-9948.	1.5	15
34	The Heaviest Possible Ternary Trihalogen Species, IAtBr^{â˜}, Evidenced in Aqueous Solution: An Experimental Performance Driven by Computations. Angewandte Chemie - International Edition, 2016, 55, 15369-15372.	7.2	15
35	Influence of ancillary ligands and solvents on the nuclearity of Niâ€“Ln complexes. Dalton Transactions, 2019, 48, 3404-3414.	1.6	13
36	Towards a Stronger Halogen Bond Involving Astatine: Unexpected Adduct with Bu₃PO Stabilized by Hydrogen Bonding. Chemistry - A European Journal, 2020, 26, 3713-3717.	1.7	13

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37	Magnetic Anisotropy in a Cubane-like Ni₄ Complex: An Ab Initio Perspective. Inorganic Chemistry, 2021, 60, 6306-6318.	1.9	13
38	Heptavalent Neptunium in a Gas-Phase Complex: (Np^{VII}O₃⁺)(NO₃^{â€“})₂. Inorganic Chemistry, 2016, 55, 9830-9837.	1.9	12
39	The bonding picture in hypervalent XF₃ (Xâ€‰=â€‰Cl, Br, I, At) fluorides revisited with quantum chemical topology. Journal of Computational Chemistry, 2017, 38, 2753-2762.	1.5	11
40	Relevance of effective bond orders in heterodiatomic molecules and role of the spin-orbit coupling in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>At</mml:mi><mml:mi>X</mml:mi></mml:mrow></mml:m xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mo>(</mml:mo><mml:mi>X</mml:mi><mml:mo>=</mml:mo><mml:mi>A	1.0	11
41	100, . Quantum chemical topology at the spinâ€“orbit configuration interaction level: Application to astatine compounds. Journal of Computational Chemistry, 2020, 41, 2055-2065.	1.5	10
42	How to create giant Dzyaloshinskiiâ€“Moriya interactions? Analytical derivation and ab initio calculations on model dicopper(II) complexes. Journal of Chemical Physics, 2021, 154, 134301.	1.2	10
43	The Heaviest Possible Ternary Trihalogen Species, IAtBr^{â˜’}, Evidenced in Aqueous Solution: An Experimental Performance Driven by Computations. Angewandte Chemie, 2016, 128, 15595-15598.	1.6	8
44	Unraveling the hydration-induced ground-state change of AtO⁺ by relativistic and multiconfigurational wave-function-based methods. Physical Chemistry Chemical Physics, 2016, 18, 32703-32712.	1.3	8
45	Extraction of giant Dzyaloshinskiiâ€“Moriya interaction from ab initio calculations: First-order spinâ€“orbit coupling model and methodological study. Journal of Chemical Physics, 2021, 155, 164305.	1.2	8
46	Zero-Field Splitting in Transition Metal Complexes: Ab Initio Calculations, Effective Hamiltonians, Model Hamiltonians, and Crystal-Field Models. , 2017, , 765-796.		7
47	An expanded halogen bonding scale using astatine. Chemical Science, 2021, 12, 10855-10861.	3.7	7
48	UVâ€“Vis Absorption Spectroscopy of Polonium(IV) Chloride Complexes: An Electronic Structure Theory Study. Inorganic Chemistry, 2019, 58, 7036-7043.	1.9	6
49	Controlling Cationâ€Cation Interactions in Uranyl Coordination Dimers by Varying the Length of the Dicarboxylate Linker. European Journal of Inorganic Chemistry, 2020, 2020, 4465-4476.	1.0	3
50	Characterization of Uranyl Coordinated by Equatorial Oxygen: Oxo in UO₃ versus Oxyl in UO₃⁺. Journal of Physical Chemistry A, 2021, 125, 5544-5555.	1.1	1
51	Zero-Field Splitting in Transition Metal Complexes: Ab Initio Calculations, Effective Hamiltonians, Model Hamiltonians, and Crystal-Field Models. , 2016, , 1-31.		1
52	Synergy and destructive interferences between local magnetic anisotropies in binuclear complexes. AIP Conference Proceedings, 2015, , .	0.3	0