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	An expanded halogen bonding scale using astatine. Chemical Science, 2021, 12, 10855-10861.	3.7	7
2	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
3	Magnetic Anisotropy in a Cubane-like Ni₄ Complex: An Ab Initio Perspective. Inorganic Chemistry, 2021, 60, 6306-6318.	1.9	13
4	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
5	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
6	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
7	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
8	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
9	Relevance of effective bond orders in heteradiatomic 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 100. ,	1.0	11
10	UVâ€“Vis Absorption Spectroscopy of Polonium(IV) Chloride Complexes: An Electronic Structure Theory Study. Inorganic Chemistry, 2019, 58, 7036-7043.	1.9	6
11	Influence of ancillary ligands and solvents on the nuclearity of Niâ€“Ln complexes. Dalton Transactions, 2019, 48, 3404-3414.	1.6	13
12	Experimental and computational evidence of halogen bonds involving astatine. Nature Chemistry, 2018, 10, 428-434.	6.6	63
13	Targeted radionuclide therapy with astatine-211: Oxidative dehalogenation of astatobenzoate conjugates. Scientific Reports, 2017, 7, 2579.	1.6	45
14	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
15	Zero-Field Splitting in Transition Metal Complexes: Ab Initio Calculations, Effective Hamiltonians, Model Hamiltonians, and Crystal-Field Models. , 2017, , 765-796.		7
16	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
17	Scrutinizing â€œInvisibleâ€•astatine: A challenge for modern density functionals. Journal of Computational Chemistry, 2016, 37, 1345-1354.	1.5	42
18	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

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19	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
20	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
21	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
22	Heptavalent Neptunium in a Gas-Phase Complex: (Np^{VII}O₃⁺)(NO₃^{â€“})₂. Inorganic Chemistry, 2016, 55, 9830-9837.	1.9	12
23	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
24	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
25	Zero-Field Splitting in Transition Metal Complexes: Ab Initio Calculations, Effective Hamiltonians, Model Hamiltonians, and Crystal-Field Models. , 2016, , 1-31.		1
26	Synergy and destructive interferences between local magnetic anisotropies in binuclear complexes. AIP Conference Proceedings, 2015, , .	0.3	0
27	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
28	Synthesis and Structures of Plutonyl Nitrate Complexes: Is Plutonium Heptavalent in PuO₃(NO₃)₂^{â€“} ?. Inorganic Chemistry, 2015, 54, 2367-2373.	1.9	19
29	Electronic structures and geometries of the XF3 (X = Cl, Br, I, At) fluorides. Journal of Chemical Physics, 2015, 143, 114306.	1.2	17
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	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
32	Unusual structure, bonding and properties in a californium borate. Nature Chemistry, 2014, 6, 387-392.	6.6	110
33	Computational determination of the dominant triplet population mechanism in photoexcited benzophenone. Physical Chemistry Chemical Physics, 2014, 16, 25393-25403.	1.3	42
34	Interplay between Local Anisotropies in Binuclear Complexes. Inorganic Chemistry, 2014, 53, 4508-4516.	1.9	36
35	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
36	Single-Ion Magnetic Anisotropy and Isotropic Magnetic Couplings in the Metalâ€“Organic Framework Fe₂(dobdc). Inorganic Chemistry, 2013, 52, 9379-9389.	1.9	43

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37	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
38	Origin of the Magnetic Anisotropy in Heptacoordinate Ni^{II} and Co^{II} Complexes. Chemistry - A European Journal, 2013, 19, 950-956.	1.7	145
39	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
40	Magnetic State of PyrochloreCd2Os2O7Emerging from Strong Competition of Ligand Distortions and Longer-Range Crystalline Anisotropy. Physical Review Letters, 2013, 110, 127206.	2.9	59
41	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
42	Magnetic interactions in LiCu2O2: Single-chain versus double-chain models. Physical Review B, 2012, 86, .	1.1	23
43	First-principles study of magnetic interactions in cupric oxide. Physical Review B, 2012, 85, .	1.1	26
44	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
45	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
46	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
47	Theoretical Determination of the Zero-Field Splitting in Copper Acetate Monohydrate. Inorganic Chemistry, 2011, 50, 6229-6236.	1.9	91
48	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
49	Antisymmetric Magnetic Interactions in Oxo-Bridged Copper(II) Bimetallic Systems. Journal of Chemical Theory and Computation, 2010, 6, 3092-3101.	2.3	51
50	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
51	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
52	Universal Theoretical Approach to Extract Anisotropic Spin Hamiltonians. Journal of Chemical Theory and Computation, 2009, 5, 2977-2984.	2.3	270