# Nathalie GuihÃ©ry

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6495044/publications.pdf

Version: 2024-02-01

| | | | |
|---|---|---|---|
| 20 papers | 1,646 citations | 516215 16 h-index | 752256 20 g-index |
| 20 all docs | 20 docs citations | 20 times ranked | 1609 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | 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 |
| 2 | Understanding the impact of correlation on bond length alternation in polyenes. Theoretical Chemistry Accounts, 2021, 140, 1. | 0.5 | 5 |
| 3 | Trinuclear Cyanidoâ€Bridged [Cr<sub>2</sub>Fe] Complexes: To Be or not to Be a Singleâ€Molecule Magnet, a Matter of Straightness. Chemistry - A European Journal, 2021, 27, 15484-15495. | 1.7 | 9 |
| 4 | 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 |
| 5 | Cyano-Bridged Fe(II)â€“Cr(III) Single-Chain Magnet Based on Pentagonal Bipyramid Units: On the Added Value of Aligned Axial Anisotropy. Journal of the American Chemical Society, 2018, 140, 7698-7704. | 6.6 | 70 |
| 6 | Pentagonal Bipyramid Fe<sup>II</sup> Complexes: Robust Isingâ€Spin Units towards Heteropolynuclear Nanomagnets. Chemistry - A European Journal, 2017, 23, 4380-4396. | 1.7 | 67 |
| 7 | Magnetic Interactions in Molecules and Highly Correlated Materials: Physical Content, Analytical Derivation, and Rigorous Extraction of Magnetic Hamiltonians. Chemical Reviews, 2014, 114, 429-492. | 23.0 | 342 |
| 8 | Interplay between Local Anisotropies in Binuclear Complexes. Inorganic Chemistry, 2014, 53, 4508-4516. | 1.9 | 36 |
| 9 | 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 |
| 10 | Origin of the Magnetic Anisotropy in Heptacoordinate Ni<sup>II</sup> and Co<sup>II</sup> Complexes. Chemistry - A European Journal, 2013, 19, 950-956. | 1.7 | 145 |
| 11 | 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 |
| 12 | A Strategy to Determine Appropriate Active Orbitals and Accurate Magnetic Couplings in Organic Magnetic Systems. Journal of Chemical Theory and Computation, 2012, 8, 4127-4137. | 2.3 | 35 |
| 13 | First-principles study of magnetic interactions in cupric oxide. Physical Review B, 2012, 85, . | 1.1 | 26 |
| 14 | Pentanuclear Cyanide-Bridged Complexes Based on Highly Anisotropic Co<sup>II</sup> Seven-Coordinate Building Blocks: Synthesis, Structure, and Magnetic Behavior. Inorganic Chemistry, 2011, 50, 12045-12052. | 1.9 | 66 |
| 15 | Theoretical Determination of the Zero-Field Splitting in Copper Acetate Monohydrate. Inorganic Chemistry, 2011, 50, 6229-6236. | 1.9 | 91 |
| 16 | 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 |
| 17 | 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 |
| 18 | Universal Theoretical Approach to Extract Anisotropic Spin Hamiltonians. Journal of Chemical Theory and Computation, 2009, 5, 2977-2984. | 2.3 | 270 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Bond electron pair: Its relevance and analysis from the quantum chemistry point of view. Journal of Computational Chemistry, 2007, 28, 35-50. | 1.5 | 64 |
| 20 | Direct generation of local orbitals for multireference treatment and subsequent uses for the calculation of the correlation energy. Journal of Chemical Physics, 2002, 116, 10060-10068. | 1.2 | 107 |