

# Mihail Atanasov

## List of Publications by Year in descending order

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34  
papers

3,571  
citations

304743

22  
h-index

414414

32  
g-index

36  
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36  
docs citations

36  
times ranked

3037  
citing authors

#	ARTICLE	IF	CITATIONS
1	First-Principles Study of Optical Absorption Energies, Ligand Field and Spin-Hamiltonian Parameters of Cr <sup>3+</sup> Ions in Emeralds. <i>Inorganic Chemistry</i> , 2022, 61, 178-192.	4.0	10
2	Robust magnetic anisotropy of a monolayer of hexacoordinate Fe(II) complexes assembled on Cu(111). <i>Inorganic Chemistry Frontiers</i> , 2021, 8, 2395-2404.	6.0	9
3	Coexistence of Two Different Distorted Octahedral [MnF <sub>6</sub> ] <sup>3-</sup> Sites in K <sub>3</sub> [MnF <sub>6</sub> ]: Manifestation in Spectroscopy and Magnetism. <i>Chemistry - A European Journal</i> , 2021, 27, 9801-9813.	3.3	11
4	Effect of Spin-Orbit Coupling on Phonon-Mediated Magnetic Relaxation in a Series of Zero-Valent Vanadium, Niobium, and Tantalum Isocyanide Complexes. <i>Inorganic Chemistry</i> , 2021, 60, 18553-18560.	4.0	15
5	Dispersion Forces Drive the Formation of Uranium-Alkane Adducts. <i>Journal of the American Chemical Society</i> , 2020, 142, 1864-1870.	13.7	17
6	Spin-chemical effects on intramolecular photoinduced charge transfer reactions in bisphenanthroline copper(I)-viologen dyad assemblies. <i>Chemical Science</i> , 2020, 11, 5511-5525.	7.4	0
7	Improvement of Ab Initio Ligand Field Theory by Means of Multistate Perturbation Theory. <i>Journal of Physical Chemistry A</i> , 2020, 124, 1025-1037.	2.5	28
8	Probing Magnetic Excitations in Coll Single-Molecule Magnets by Inelastic Neutron Scattering. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 1055-1055.	2.0	0
9	Probing Magnetic Excitations in Co(II) Single-Molecule Magnets by Inelastic Neutron Scattering. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 1119-1127.	2.0	14
10	Chemistry and Quantum Mechanics in 2019: Give Us Insight <i>and</i> Numbers. <i>Journal of the American Chemical Society</i> , 2019, 141, 2814-2824.	13.7	93
11	The [U <sub>2</sub> F <sub>12</sub> ] <sup>2-</sup> Anion of Sr[U <sub>2</sub> F <sub>12</sub> ]. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 2914-2918.	13.8	11
12	A linear cobalt(II) complex with maximal orbital angular momentum from a non-Aufbau ground state. <i>Science</i> , 2018, 362, .	12.6	254
13	Computational Studies on Vibronic Coupling in Single Molecule Magnets: Impact on the Mechanism of Magnetic Relaxation. <i>Journal of Physics: Conference Series</i> , 2018, 1148, 012006.	0.4	8
14	Spin-phonon couplings in transition metal complexes with slow magnetic relaxation. <i>Nature Communications</i> , 2018, 9, 2572.	12.8	93
15	Challenges in Multireference Perturbation Theory for the Calculations of the <i>g</i> -Tensor of First-Row Transition-Metal Complexes. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4662-4677.	5.3	55
16	Magneto-Structural Correlations in Pseudotetrahedral Forms of the [Co(SPh) <sub>4</sub> ] <sup>2-</sup> Complex Probed by Magnetometry, MCD Spectroscopy, Advanced EPR Techniques, and ab Initio Electronic Structure Calculations. <i>Inorganic Chemistry</i> , 2017, 56, 3102-3118.	4.0	74
17	Covalency and chemical bonding in transition metal complexes: An ab initio based ligand field perspective. <i>Coordination Chemistry Reviews</i> , 2017, 344, 2-25.	18.8	178
18	Ab Initio Ligand-Field Theory Analysis and Covalency Trends in Actinide and Lanthanide Free Ions and Octahedral Complexes. <i>Inorganic Chemistry</i> , 2017, 56, 8802-8816.	4.0	106

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19	Measurement of the Ligand Field Spectra of Ferrous and Ferric Iron Chlorides Using 2p3d RIXS. <i>Inorganic Chemistry</i> , 2017, 56, 8203-8211.	4.0	15
20	Periodic Trends in Lanthanide Compounds through the Eyes of Multireference ab Initio Theory. <i>Inorganic Chemistry</i> , 2016, 55, 4457-4469.	4.0	98
21	A four-coordinate cobalt(II) single-ion magnet with coercivity and a very high energy barrier. <i>Nature Communications</i> , 2016, 7, 10467.	12.8	374
22	Magnetic Transitions in Iron Porphyrin Halides by Inelastic Neutron Scattering and Ab Initio Studies of Zero-Field Splittings. <i>Inorganic Chemistry</i> , 2015, 54, 9790-9801.	4.0	49
23	First principles approach to the electronic structure, magnetic anisotropy and spin relaxation in mononuclear 3d-transition metal single molecule magnets. <i>Coordination Chemistry Reviews</i> , 2015, 289-290, 177-214.	18.8	267
24	Slow magnetization dynamics in a series of two-coordinate iron(II) complexes. <i>Chemical Science</i> , 2013, 4, 125-138.	7.4	518
25	A theoretical analysis of chemical bonding, vibronic coupling, and magnetic anisotropy in linear iron(II) complexes with single-molecule magnet behavior. <i>Chemical Science</i> , 2013, 4, 139-156.	7.4	243
26	Magnetic blocking in a linear iron(I) complex. <i>Nature Chemistry</i> , 2013, 5, 577-581.	13.6	562
27	Mössbauer Spectroscopy as a Probe of Magnetization Dynamics in the Linear Iron(I) and Iron(II) Complexes $[\text{Fe}(\text{C}(\text{SiMe}_3)_2)_2]^{+}$ . <i>Inorganic Chemistry</i> , 2013, 52, 13123-13131.	4.0	99
28	A Modern First-Principles View on Ligand Field Theory Through the Eyes of Correlated Multireference Wavefunctions. <i>Structure and Bonding</i> , 2011, , 149-220.	1.0	94
29	Combined Ligand Field and Density Functional Theory Analysis of the Magnetic Anisotropy in Oligonuclear Complexes Based on $\text{Fe}^{\text{III}}/\text{M}^{\text{II}}$ Exchange-Coupled Pairs. <i>Inorganic Chemistry</i> , 2008, 47, 2449-2463.	4.0	78
30	Trinuclear $\{\text{M}^{\text{I}}\}_2\text{CN}\{\text{M}^{\text{II}}\}_2$ Complexes ( $\text{M}^{\text{I}} = \text{Tl}, \text{Pb}, \text{Bi}, \text{Po}, \text{At}, \text{Fr}$ ). <i>Inorganic Chemistry</i> , 2007, 46, 1000-1006.	4.0	60
31	DFT Studies on the Magnetic Exchange Across the Cyanide Bridge. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13332-13340.	2.5	55
32	Chemical Bonding in Molecules and Complexes Containing d-Elements Based on DFT. <i>Monatshefte für Chemie</i> , 2005, 136, 925-963.	1.8	11
33	Calculation of spin-orbit coupling within the LFDFT: Applications to $[\text{NiX}_4]^{2-}$ ( $X = \text{F}, \text{Cl}, \text{Br}, \text{I}$ ). <i>International Journal of Quantum Chemistry</i> , 2005, 102, 119-131.	2.0	48
34	On the Mechanism of Indeno[1,2,3-c,d]-pyrene Ozonation. <i>Monatshefte für Chemie</i> , 1998, 129, 999-1005.	1.8	0