

Computational design of magnetic molecules and their chemistry, machine learning and multiscale simulation

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Unraveling the Contributions to Spin-Lattice Relaxation in Kramers Single-Molecule Magnets. Journal of the American Chemical Society, 2022, 144, 22965-22975.	13.7	21
2	Data-driven design of molecular nanomagnets. Nature Communications, 2022, 13, .	12.8	12
3	Machine Learning Predicting Optimal Preparation of Silica-Coated Gold Nanorods for Photothermal Tumor Ablation. Nanomaterials, 2023, 13, 1024.	4.1	4
4	Machine learning for new material prediction, what's next?. , 2023, 1, 100005.		1
5	The critical role of ultra-low-energy vibrations in the relaxation dynamics of molecular qubits. Nature Communications, 2023, 14, .	12.8	6
6	Ab initio prediction of key parameters and magneto-structural correlation of tetracoordinated lanthanide single-ion magnet. Physical Chemistry Chemical Physics, 0, , .	2.8	3
7	Get under the Umbrella: A Comprehensive Gateway for Researchers on Lanthanide-Based Single-Molecule Magnets. European Journal of Inorganic Chemistry, 2023, 26, .	2.0	4
8	Spin-Phonon Relaxation in Magnetic Molecules: Theory, Predictions and Insights. Challenges and Advances in Computational Chemistry and Physics, 2023, , 219-289.	0.6	6
9	Noncanonical Condensation of Nucleic Acid Chains by Hydrophobic Gold Nanocrystals. JACS Au, 2023, 3, 2206-2215.	7.9	1
10	Contribution of molecular structures and quantum chemistry technique to root concentration factor: An innovative application of interpretable machine learning. Journal of Hazardous Materials, 2023, 459, 132320.	12.4	0
11	Semi-empirical Haken-Strobl model for molecular spin qubits. New Journal of Physics, 2023, 25, 093031.	2.9	0
12	Rapid and Accurate Prediction of the Axial Magnetic Anisotropy in Cobalt(II) Complexes Using a Machine-Learning Approach. Inorganic Chemistry, 2023, 62, 14838-14842.	4.0	0
13	Lanthanide molecular nanomagnets as probabilistic bits. Npj Computational Materials, 2023, 9, .	8.7	1
14	Triplet-mediated spin entanglement between organic radicals: integrating first principles and open-quantum-system simulations. NPG Asia Materials, 2023, 15, .	7.9	1
15	Accelerating search for the polar phase stability of ferroelectric oxide by machine learning. Materials and Design, 2023, 236, 112518.	7.0	0
16	First-principles study of structure and bonding in Ni-group transition metal carbonyls with terminal tin chalcogenides $[M(CO)_3 SnX]$ ($M = Ni, Pd, Pt$; $X = O, S, Se, \text{ and } Te$) complexes. Molecular Physics, 0, , .		0
17	High-performance molecular spin filters based on a square-planar four-coordinate Fe complex and covalent pyrazine anchoring groups. Journal of Materials Chemistry C, 0, , .	5.5	0
18	Machine Learning Prediction of the Experimental Transition Temperature of Fe(II) Spin-Crossover Complexes. Journal of Physical Chemistry A, 0, , .	2.5	0

#	ARTICLE	IF	CITATIONS
19	Can Molecular Quantum Computing Bridge Quantum Biology and Cognitive Science?. , 2024, 3, .		0
20	Nanostructured Design Cathode Materials for Magnesium-Ion Batteries. ACS Omega, 2024, 9, 4229-4245.	3.5	0
21	Two dysprosium single molecule magnets with planar skeleton built from edge-shared Dy ₃ triangles. Journal of Molecular Structure, 2024, 1308, 138038.	3.6	0