

Karin Fink

List of Publications by Year in descending order

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papers

3,470
citations

147801

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all docs

97
docs citations

97
times ranked

5693
citing authors

#	ARTICLE	IF	CITATIONS
1	Development and Application of a Complete Active Space Spin-Orbit Configuration Interaction Program Designed for Single Molecule Magnets. <i>ChemPhysChem</i> , 2022, 23, .	2.1	10
2	The Adsorption of Small Molecules on the Copper Paddle-Wheel: Influence of the Multi-Reference Ground State. <i>Molecules</i> , 2022, 27, 912.	3.8	2
3	Asymmetrically Difunctionalized 1,1'-Ferrocenyl Metalloligands and Their Transition Metal Complexes. <i>European Journal of Inorganic Chemistry</i> , 2022, 2022, .	2.0	1
4	Tuning the Coordination Geometry and Magnetic Relaxation of Co(II) Single-Ion Magnets by Varying the Ligand Substitutions. <i>Crystal Growth and Design</i> , 2021, 21, 1035-1044.	3.0	13
5	Combining wavefunction frozen-density embedding with one-dimensional periodicity. <i>Journal of Chemical Physics</i> , 2021, 154, 104114.	3.0	4
6	Heterobimetallic Lanthanide-Coinage Metal Compounds Featuring Possible Metal-Metal Interactions in the Excited State. <i>Chemistry - A European Journal</i> , 2021, 27, 15128-15136.	3.3	12
7	Terminal Ligand and Packing Effects on Slow Relaxation in an Isostructural Set of [Dy(H ₂ dpp)X ₂] ⁺ Single Molecule Magnets**. <i>Chemistry - A European Journal</i> , 2021, 27, 15086-15095.	3.3	6
8	Frontispiece: Terminal Ligand and Packing Effects on Slow Relaxation in an Isostructural Set of [Dy(H ₂ dpp)X ₂] ⁺ Single Molecule Magnets. <i>Chemistry - A European Journal</i> , 2021, 27, .	3.3	0
9	Formation and desorption of nickel hexafluoroacetylacetonate Ni(hfac) ₂ on a nickel oxide surface in atomic layer etching processes. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2020, 38, .	2.1	12
10	Rational Design of Iron Oxide Binding Peptide Tags. <i>Langmuir</i> , 2019, 35, 8472-8481.	3.5	5
11	Photodissociation of Free Metalloporphyrin Dimer Multianions. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2974-2982.	2.5	8
12	Gas-Phase Ion Chemistry of Metalloporphyrin Anions with Molecular Oxygen: Probing the Influence of the Oxidation and Spin State of the Central Transition Metal by Experiment and Theory. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4357-4365.	2.5	8
13	Experimental characterization and simulation of amino acid and peptide interactions with inorganic materials. <i>Engineering in Life Sciences</i> , 2018, 18, 84-100.	3.6	26
14	Exploiting Synergies in Catalysis and Gas Sensing using Noble Metal-Loaded Oxide Composites. <i>ChemCatChem</i> , 2018, 10, 864-880.	3.7	50
15	Enhanced etching of tin-doped indium oxide due to surface modification by hydrogen ion injection. <i>Japanese Journal of Applied Physics</i> , 2018, 57, 06JC05.	1.5	8
16	Enantiopure Benzamidinate/Cyclooctatetraene Complexes of the Rare-Earth Elements: Synthesis, Structure, and Magnetism. <i>Organometallics</i> , 2018, 37, 3708-3717.	2.3	14
17	Mononuclear and dinuclear heteroleptic Cu(I) complexes based on pyridyl-triazole and DPEPhos with long-lived excited-state lifetimes. <i>Journal of Organometallic Chemistry</i> , 2018, 871, 140-149.	1.8	13
18	Metal Complexes of a Redox-Active [1]Phosphaferrocenophane: Structures, Electrochemistry and Redox-Induced Catalysis. <i>Chemistry - A European Journal</i> , 2017, 23, 7402-7408.	3.3	35

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19	Effects of hydrogen ion irradiation on zinc oxide etching. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2017, 35, .	2.1	13
20	Field-Induced Co(II) Single-Ion Magnets with <i>mer</i> -Directing Ligands but Ambiguous Coordination Geometry. <i>Inorganic Chemistry</i> , 2017, 56, 6056-6066.	4.0	35
21	Binding patterns of homo-peptides on bare magnetic nanoparticles: insights into environmental dependence. <i>Scientific Reports</i> , 2017, 7, 14047.	3.3	25
22	Defects as Color Centers: The Apparent Color of Metal-Organic Frameworks Containing Cu ²⁺ -Based Paddle-Wheel Units. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 37463-37467.	8.0	60
23	Toward On-Off Magnetism: Reversible Electrochemistry to Control Magnetic Phase Transitions in Spinel Ferrites. <i>Advanced Functional Materials</i> , 2016, 26, 7507-7515.	14.9	69
24	Magnetic anisotropy of a Co ^{II} single ion magnet with distorted trigonal prismatic coordination: theory and experiment. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 30135-30143.	2.8	56
25	Divergent Coordination Chemistry: Parallel Synthesis of [2-2] Iron(II) Grid-Complex Tauto-Conformers. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 10881-10885.	13.8	41
26	Carbon incorporation effects and reaction mechanism of FeOCl cathode materials for chloride ion batteries. <i>Scientific Reports</i> , 2016, 6, 19448.	3.3	43
27	Field-Induced Slow Magnetic Relaxation in the Ni(I) Complexes [NiCl(PPH ₃) ₂] ₂ ·C ₄ H ₈ O and [Ni(N(SiMe ₃) ₂)(PPH ₃) ₂]. <i>Inorganic Chemistry</i> , 2016, 55, 2091-2100.	4.0	73
28	A fascinating multifaceted redox-active chelating ligand: introducing the N,N'-dimethyl-3,3'-biquinoxalium <i>æ</i> methylbiquinoxen ⁺ platform. <i>Chemical Science</i> , 2016, 7, 3820-3828. ^{7.4}		8
29	Q and Soret Band Photoexcitation of Isolated Palladium Porphyrin Tetraanions Leads to Delayed Emission of Nonthermal Electrons over Microsecond Time Scales. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1167-1172.	4.6	19
30	Interaction of carboxylic acids with rutile TiO ₂ (110): IR-investigations of terephthalic and benzoic acid adsorbed on a single crystal substrate. <i>Surface Science</i> , 2016, 643, 117-123.	1.9	39
31	Band-gap engineering with a twist: Formation of intercalant superlattices in twisted graphene bilayers. <i>Physical Review B</i> , 2015, 91, .	3.2	18
32	Ab initio calculations on the magnetic properties of transition metal complexes. <i>AIP Conference Proceedings</i> , 2015, , .	0.4	0
33	Experimental and theoretical investigations of the electronic band structure of metal-organic frameworks of HKUST-1 type. <i>Applied Physics Letters</i> , 2015, 107, .	3.3	57
34	Tris(3,5-dimethylpyrazolyl)methane-Based Heterobimetallic Complexes that Contain Zn ^{II} and Cd ^{II} Transition-Metal Bonds: Synthesis, Structures, and Quantum Chemical Calculations. <i>Chemistry - A European Journal</i> , 2015, 21, 2905-2914.	3.3	19
35	Interfacial dominated ferromagnetism in nanograined ZnO: a ¹ / ₄ SR and DFT study. <i>Scientific Reports</i> , 2015, 5, 8871.	3.3	97
36	The Interaction of Formic Acid with Zinc Oxide: A Combined Experimental and Theoretical Study on Single Crystal and Powder Samples. <i>Topics in Catalysis</i> , 2015, 58, 174-183.	2.8	32

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37	Ab Initio Study of the Adsorption of Small Molecules on Metal-Organic Frameworks with Oxo-centered Trimetallic Building Units: The Role of the Undercoordinated Metal Ion. <i>Inorganic Chemistry</i> , 2015, 54, 8251-8263.	4.0	48
38	Bi- and trimetallic rare-earth-palladium complexes ligated by phosphinoamides. <i>Chemical Communications</i> , 2015, 51, 11761-11764.	4.1	26
39	Trinuclear Early/Late-Transition-Metal Thiolate Complexes. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 3510-3520.	2.0	6
40	Cu(II)- and Mn(III)-Porphyrin-Derived Oligomeric Multianions: Structures and Photoelectron Spectra. <i>Journal of Physical Chemistry A</i> , 2014, 118, 369-379.	2.5	13
41	Spin-Crossover and Massive Anisotropy Switching of 5d Transition Metal Atoms on Graphene Nanoflakes. <i>Nano Letters</i> , 2014, 14, 3364-3368.	9.1	28
42	Magnesium Anode for Chloride Ion Batteries. <i>ACS Applied Materials & Interfaces</i> , 2014, 6, 10997-11000.	8.0	69
43	Switching of a coupled spin pair in a single-molecule junction. <i>Nature Nanotechnology</i> , 2013, 8, 575-579.	31.5	107
44	A modified CAS-Cl approach for an efficient calculation of magnetic exchange coupling constants. <i>Molecular Physics</i> , 2013, 111, 2594-2605.	1.7	15
45	Catalytic subsurface etching of nanoscale channels in graphite. <i>Nature Communications</i> , 2013, 4, 1379.	12.8	46
46	Magnetic anisotropy of graphene quantum dots decorated with a ruthenium adatom. <i>Beilstein Journal of Nanotechnology</i> , 2013, 4, 441-445.	2.8	4
47	Interkingdom Signaling: Integration, Conformation, and Orientation of N-Acyl-homoserine Lactones in Supported Lipid Bilayers. <i>Langmuir</i> , 2012, 28, 8456-8462.	3.5	27
48	[2.2]Paracyclophane derived bisphosphines for the activation of hydrogen by FLPs: application in domino hydrosilylation/hydrogenation of enones. <i>Dalton Transactions</i> , 2012, 41, 9056.	3.3	58
49	Selective Coordination Bonding in Metallo-Supramolecular Systems on Surfaces. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 4327-4331.	13.8	40
50	The Surface Science Approach for Understanding Reactions on Oxide Powders: The Importance of IR Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 4731-4734.	13.8	68
51	Theoretical Approach Towards the Understanding of Asymmetric Additions of Dialkylzinc to Enals and Iminals Catalysed by [2.2]Paracyclophane-Based N,O-Ligands. <i>Chemistry - A European Journal</i> , 2012, 18, 8377-8385.	3.3	10
52	Deuterium-labelled N-acyl-homoserine lactones (AHLs) inter-kingdom signalling molecules synthesis, structural studies, and interactions with model lipid membranes. <i>Analytical and Bioanalytical Chemistry</i> , 2012, 403, 473-482.	3.7	14
53	Homoleptic 1-D iron selenolate complexes synthesis, structure, magnetic and thermal behaviour of $1\text{-D}[\text{Fe}(\text{SeR})_2]$ (R = Ph, Mes). <i>Dalton Transactions</i> , 2011, 40, 7022.	3.3	29
54	How molecular oxygen binds to bis[trifluoroacetylacetonato(η^1)]cobalt(ii) ab initio and density functional theory studies. <i>Dalton Transactions</i> , 2011, 40, 11289.	3.3	10

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55	Size and Isotope Effects of Helium Clusters and Droplets: Identification of Surface and Bulk-Volume Excitations. <i>Journal of Physical Chemistry A</i> , 2011, 115, 7316-7326.	2.5	31
56	The Formal Combination of Three Singlet Biradicaloid Entities to a Singlet Hexaradicaloid Metalloid $\text{Ge}_{14}[\text{Si}(\text{SiMe}_3)_3]_3[\text{Li}(\text{THF})_2]_3$ Cluster. <i>Journal of the American Chemical Society</i> , 2011, 133, 2518-2524.	13.7	49
57	Charge Density Analysis of 2-Methyl-4-nitro-1-phenyl-1H-imidazole-5-carbonitrile: An Experimental and Theoretical Study of $\text{C}\cdots\text{N}\cdots\text{N}$ Interactions. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12941-12952.	2.5	21
58	Electrical control over the Fe(II) spin crossover in a single molecule: Theory and experiment. <i>Physical Review B</i> , 2011, 83, .	3.2	169
59	Uniform π -System Alignment in Thin Films of Template-Grown Dicarbonitrile-Oligophenyls. <i>Advanced Functional Materials</i> , 2011, 21, 1631-1642.	14.9	32
60	Magnetic Properties of Paddlewheels and Trinuclear Clusters with Exposed Metal Sites. <i>ChemPhysChem</i> , 2011, 12, 3307-3319.	2.1	27
61	$[\text{Sn}_4\text{Si}\{\text{Si}(\text{SiMe}_3)_3\}_4\{\text{SiMe}_3\}_2]$: A Model Compound for the Unexpected First-Order Transition from a Singlet Biradicaloid to a Classical Bonded Molecule. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 7273-7277.	13.8	17
62	Density-functional study on the migration of Cd and Te adsorbates on the (001) surface of CdTe. <i>Physica Status Solidi (B): Basic Research</i> , 2010, 247, 937-944.	1.5	3
63	NMR-Spectroscopic and Solid-State Investigations of Cometal-Free Asymmetric Conjugate Addition: A Dinuclear Paracyclophaneimine Zinc Methyl Complex. <i>Journal of the American Chemical Society</i> , 2010, 132, 12899-12905.	13.7	29
64	Expanding the Coordination Cage: A Ruthenium(II)-Polypyridine Complex Exhibiting High Quantum Yields under Ambient Conditions. <i>Inorganic Chemistry</i> , 2009, 48, 5677-5684.	4.0	73
65	Synthesis, Electronic Structure, and Structural Characterization of the New, π -Non-Innocent 4,5-Dithio-Catecholate Ligand, Its Metal Complexes, and Their Oxidized 4,5-Dithio-quinone Derivatives. <i>Inorganic Chemistry</i> , 2009, 48, 8830-8844.	4.0	14
66	Synthesis and Structure of an Iron-Doped Copper Selenide Cluster Molecule: $[\text{Cu}_{30}\text{Fe}_2\text{Se}_6(\text{SePh})_{24}(\text{dppm})_4]$. <i>Inorganic Chemistry</i> , 2009, 48, 8977-8984.	4.0	19
67	The method of local increments for the calculation of adsorption energies of atoms and small molecules on solid surfaces : Part I. A single Cu atom on the polar surfaces of ZnO. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 11196.	2.8	25
68	Ab initio study of the magnetic exchange coupling constants of a structural model $[\text{CaMn}_3\text{MnII}]$ of the oxygen evolving center in photosystem II. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 3900.	2.8	23
69	Adsorption of single Cu atoms at differently stabilized polar ZnO surfaces: An <i>ab initio</i> study. <i>Journal of Computational Chemistry</i> , 2008, 29, 2302-2310.	3.3	13
70	Lithium-promoted hydrogenation of carbon dioxide to formates by heterobimetallic hydrido zinc alkoxide clusters. <i>Chemical Communications</i> , 2008, , 73-75.	4.1	25
71	The spin coupling in the diiron complex $[\text{Fe}_2(\text{hpdt})(\text{H}_2\text{O})_3\text{Cl}]$. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 1911-1920.	2.8	13
72	A quantum chemical approach towards the electronically excited states of helium clusters. <i>European Physical Journal D</i> , 2007, 43, 121-124.	1.3	12

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73	Ab initio cluster calculations on the electronic structure of oxygen vacancies at the polar ZnO(0001̄,,) surface and on the adsorption of H ₂ , CO, and CO ₂ at these sites. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 1482.	2.8	46
74	Ab initio cluster calculations of the magnetic properties of ZnO doped with transition metal ions. <i>Chemical Physics</i> , 2006, 326, 297-307.	1.9	20
75	Active Sites on Oxide Surfaces: ZnO-Catalyzed Synthesis of Methanol from CO and H ₂ . <i>Angewandte Chemie - International Edition</i> , 2005, 44, 2790-2794.	13.8	192
76	Zinc Oxide Nanoparticles with Defects. <i>Advanced Functional Materials</i> , 2005, 15, 1945-1954.	14.9	499
77	Ab initio Cluster Calculations for the Absorption Energies of F and F ⁺ Centers in Bulk ZnO.. <i>ChemInform</i> , 2005, 36, no.	0.0	0
78	Comment on "Excitations in photoactive molecules from quantum Monte Carlo" [J. Chem. Phys. 121, 5836 (2004)]. <i>Journal of Chemical Physics</i> , 2005, 122, 087101.	3.0	6
79	Ab initio cluster calculations for the absorption energies of F and F ⁺ centers in bulk ZnO. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 2999.	2.8	31
80	Stabilization of Polar ZnO Surfaces: Validating Microscopic Models by Using CO as a Probe Molecule. <i>Physical Review Letters</i> , 2003, 90, 106102.	7.8	164
81	An ab initio study of the adsorption of CO on a Zn ₄ O ₄ cluster with wurtzite-like structure. <i>Chemical Physics</i> , 2003, 287, 183-195.	1.9	24
82	An ab initio cluster study of the magnetic properties of the CoO(001) surface. <i>Chemical Physics</i> , 2002, 278, 79-87.	1.9	27
83	Ab initio calculation of the magnetic exchange coupling in linear oxo-bridged heterobinuclear complexes of titanium (III), vanadium (III), and chromium (III). <i>International Journal of Quantum Chemistry</i> , 2000, 76, 137-147.	2.0	21
84	Superexchange and Spin [↗] Orbit Coupling in Chlorine-Bridged Binuclear Cobalt(II) Complexes. <i>Inorganic Chemistry</i> , 1999, 38, 3847-3856.	4.0	59
85	Ab initio calculation of potential energy surfaces for the three lowest triplet states (1 [↗] 3A [↗] 2 [↗] , 1 [↗] 3A [↗] 2 [↗] , 3 [↗] A [↗] 2 [↗]) of PH(X,A)He. <i>Journal of Chemical Physics</i> , 1997, 106, 7637-7641.	3.0	4
86	Autoionization spectroscopy of CO on metal oxide surfaces. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 1996, 77, 155-171.	1.7	7
87	A quantum chemical ab initio study of the superexchange coupling in binuclear oxygen-bridged Ni(II) complexes. <i>Chemical Physics</i> , 1995, 192, 25-35.	1.9	50
88	An ab initio study of the geometry dependence of the magnetic exchange coupling in oxo-bridged binuclear chromium(III) complexes. <i>Chemical Physics</i> , 1995, 201, 87-94.	1.9	39
89	Ab initio calculations of van der Waals interactions in one- and two-dimensional infinite periodic systems. <i>Journal of Chemical Physics</i> , 1995, 103, 2603-2614.	3.0	26
90	Ab Initio Calculation of the Magnetic Exchange Coupling in Linear Oxo-Bridged Binuclear Complexes of Titanium(III), Vanadium(III), and Chromium(III). <i>Inorganic Chemistry</i> , 1994, 33, 6219-6229.	4.0	89