Carmen Herrmann

List of Publications by Year in descending order

79 papers	2,466 citations	218592 26 h-index	214721 47 g-index
96 all docs	96 docs citations	96 times ranked	2567 citing authors

#	Article	IF	Citations
1	Exploring local currents in molecular junctions. Nature Chemistry, 2010, 2, 223-228.	6.6	375
2	Organic Radicals As Spin Filters. Journal of the American Chemical Society, 2010, 132, 3682-3684.	6.6	183
3	Ghost transmission: How large basis sets can make electron transport calculations worse. Journal of Chemical Physics, 2010, 132, 024103.	1.2	90
4	Comparative analysis of local spin definitions. Journal of Chemical Physics, 2005, 122, 034102.	1.2	87
5	The Chameleonic Nature of Electron Transport through Ï€-Stacked Systems. Journal of the American Chemical Society, 2010, 132, 7887-7889.	6.6	79
6	Large Magnetoresistance in Single-Radical Molecular Junctions. Nano Letters, 2016, 16, 4960-4967.	4.5	75
7	A Chirality-Based Quantum Leap. ACS Nano, 2022, 16, 4989-5035.	7.3	74
8	Can Raman Optical Activity Separate Axial from Local Chirality? A Theoretical Study of Helical Deca-Alanine. ChemPhysChem, 2006, 7, 2189-2196.	1.0	71
9	Finding a needle in a haystack: direct determination of vibrational signatures in complex systems. New Journal of Chemistry, 2007, 31, 818.	1.4	66
10	Trinuclear Copper(II) Complexes Derived from Schiff-Base Ligands Based on a 6-Amino-6-deoxyglucopyranoside:â€‰ Structural and Magnetic Characterization. Inorganic Chemistry, 2006, 45, 10066-10076.	1.9	64
11	Insight into the Origin of Chiral-Induced Spin Selectivity from a Symmetry Analysis of Electronic Transmission. Journal of Chemical Theory and Computation, 2020, 16, 2914-2929.	2.3	60
12	M<scp>O</scp>V<scp>I</scp>P<scp>AC</scp>: Vibrational spectroscopy with a robust metaâ€program for massively parallel standard and inverse calculations. Journal of Computational Chemistry, 2012, 33, 2186-2198.	1.5	59
13	The First Photoexcitation Step of Ruthenium-Based Models for Artificial Photosynthesis Highlighted by Resonance Raman Spectroscopy. Journal of Physical Chemistry B, 2007, 111, 6078-6087.	1.2	57
14	The Electronic Structure of the Tris(ethylene) Complexes [M(C₂H₄)₃] (M=Ni, Pd, and Pt): A Combined Experimental and Theoretical Study. Chemistry - A European Journal, 2007, 13, 10078-10087.	1.7	57
15	First-Principles Approach to Vibrational Spectroscopy of Biomolecules. , 2006, , 85-132.		56
16	Spin states in polynuclear clusters: The [Fe2O2] core of the methane monooxygenase active site. Journal of Computational Chemistry, 2006, 27, 1223-1239.	1.5	54
17	Designing organic spin filters in the coherent tunneling regime. Journal of Chemical Physics, 2011, 134, 224306.	1.2	47
18	Relevance of the Electric-Dipoleâ"Electric-Quadrupole Contribution to Raman Optical Activity Spectra. Journal of Physical Chemistry B, 2008, 112, 2218-2232.	1.2	46

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19	Cobalt-Catalyzed Hydrogenations via Olefin Cobaltate and Hydride Intermediates. ACS Catalysis, 2019, 9, 7596-7606.	5.5	46
20	Spinâ€“Spin interactions in polynuclear transition-metal complexes. Chemical Physics Letters, 2008, 451, 301-308.	1.2	36
21	Importance of backbone angles versus amino acid configurations in peptide vibrational Raman optical activity spectra. Chemical Physics, 2008, 343, 200-209.	0.9	32
22	Understanding Coherent Transport through Ï€-Stacked Systems upon Spatial Dislocation. Journal of Physical Chemistry B, 2010, 114, 14735-14744.	1.2	32
23	Electronic communication through molecular bridges. Chemical Communications, 2013, 49, 10456.	2.2	32
24	Influence of Electronic Structure Modeling and Junction Structure on First-Principles Chiral Induced Spin Selectivity. Journal of Chemical Theory and Computation, 2020, 16, 7357-7371.	2.3	31
25	Theoretical Study on the Spin-State Energy Splittings and Local Spin in Cationic [Re]â‹¯Cnâ‹¯[Re] Complexes. Inorganic Chemistry, 2005, 44, 6174-6182.	1.9	28
26	A Greenâ€™s-Function Approach to Exchange Spin Coupling As a New Tool for Quantum Chemistry. Journal of Chemical Theory and Computation, 2015, 11, 5651-5664.	2.3	27
27	Controlling Molecular Conductance: Switching Off Ï€ Sites through Protonation. ChemPhysChem, 2014, 15, 4011-4018.	1.0	26
28	Towards colloidal spintronics through Rashba spin-orbit interaction in lead sulphide nanosheets. Nature Communications, 2017, 8, 15721.	5.8	26
29	Optical and Vibrational Properties of Toroidal Carbon Nanotubes. Chemistry - A European Journal, 2011, 17, 3868-3875.	1.7	25
30	Electronic Communication as a Transferable Property of Molecular Bridges?. Journal of Physical Chemistry A, 2019, 123, 10205-10223.	1.1	25
31	Restrained optimization of brokenâ€symmetry determinants. International Journal of Quantum Chemistry, 2009, 109, 2430-2446.	1.0	24
32	Molecular Electronic Junction Transport: Some Pathways and Some Ideas. Topics in Current Chemistry, 2011, 313, 1-38.	4.0	22
33	QM/MM vibrational mode tracking. Journal of Computational Chemistry, 2008, 29, 2460-2470.	1.5	21
34	Local Pathways in Coherent Electron Transport through Iron Porphyrin Complexes: A Challenge for First-Principles Transport Calculations. Journal of Physical Chemistry C, 2010, 114, 20813-20820.	1.5	21
35	Emergence of Metallic Conduction and Cobalt(II)-Based Single-Molecule Magnetism in the Same Temperature Range. Journal of the American Chemical Society, 2021, 143, 4891-4895.	6.6	21
36	Charge Delocalization in an Organic Mixed Valent Bithiophene Is Greater Than in a Structurally Analogous Biselenophene. Journal of Physical Chemistry A, 2014, 118, 11293-11303.	1.1	20

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37	Direct targeting of adsorbate vibrations with mode-tracking. Surface Science, 2006, 600, 1891-1900.	0.8	19
38	Increasing Magnetic Coupling through Oxidation of a Ferrocene Bridge. Inorganic Chemistry, 2015, 54, 11733-11740.	1.9	19
39	Communication through molecular bridges: Different bridge orbital trends result in common property trends. Journal of Computational Chemistry, 2015, 36, 201-209.	1.5	18
40	High-conductance surface-anchoring of a mechanically flexible platform-based porphyrin complex. New Journal of Physics, 2015, 17, 013012.	1.2	17
41	Performance of rangeâ€separated hybrid exchangeâ€“correlation functionals for the calculation of magnetic exchange coupling constants of organic diradicals. Journal of Computational Chemistry, 2018, 39, 780-787.	1.5	17
42	Design Considerations for Oligo(p-phenyleneethynylene) Organic Radicals in Molecular Junctions. Journal of Physical Chemistry C, 2021, 125, 1208-1220.	1.5	17
43	Exchange Spin Coupling from Gaussian Process Regression. Journal of Physical Chemistry A, 2020, 124, 8708-8723.	1.1	16
44	Influence of Radical Bridges on Electron Spin Coupling. Journal of Physical Chemistry A, 2017, 121, 216-225.	1.1	14
45	Controlling Throughâ€Space and Throughâ€Bond Exchange Pathways in Bisâ€Cobaltocenes for Molecular Spintronics. Angewandte Chemie - International Edition, 2020, 59, 2407-2413.	7.2	14
46	Synthesis and Molecular Structures of Monosubstituted Pentamethylcobaltocenium Cations. European Journal of Inorganic Chemistry, 2014, 2014, 4115-4122.	1.0	13
47	Quantum Chemical Calculations and Experimental Validation of the Photoclick Reaction for Fluorescent Labeling of the 5â€™ cap of Eukaryotic mRNAs. ChemistryOpen, 2015, 4, 295-301.	0.9	13
48	Simultaneous manifestation of metallic conductivity and single-molecule magnetism in a layered molecule-based compound. Chemical Science, 2020, 11, 11154-11161.	3.7	13
49	Spectroscopic Investigation of a Metalâ€“Metal-Bonded Fe₆ Single-Molecule Magnet with an Isolated S = ¹⁹/₂ Giant-Spin Ground State. Inorganic Chemistry, 2021, 60, 4610-4622.	1.9	13
50	Synthesis, Structures, and Magnetic Properties of Nâ€Trialkylsilylâ€8â€amidoquinoline Complexes of Chromium, Manganese, Iron, and Cobalt as well as of Wheelâ€Like Hexanuclear Iron(II) and Manganese(II) Bis(8â€amidoquinoline). European Journal of Inorganic Chemistry, 2010, 2010, 1777-1790.	1.0	12
51	Modeâ€tracking based stationaryâ€point optimization. Journal of Computational Chemistry, 2015, 36, 1429-1438.	1.5	12
52	Toward an automated analysis of exchange pathways in spinâ€coupled systems. Journal of Computational Chemistry, 2018, 39, 81-92.	1.5	10
53	Designing Long-Range Charge Delocalization from First-Principles. Journal of Chemical Theory and Computation, 2019, 15, 165-177.	2.3	10
54	Interplay between Magnetoresistance and Kondo Resonance in Radical Single-Molecule Junctions. Nano Letters, 2022, 22, 5773-5779.	4.5	10

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55	Kondo screening in Co adatoms with full Coulomb interaction. Physical Review Research, 2020, 2, .	1.3	9
56	Photoswitching Behavior of a Cyclohexeneâ€Bridged versus a Cyclopenteneâ€Bridged Dithienylethene System. ChemPhysChem, 2015, 16, 1491-1501.	1.0	8
57	Interplay between strong correlation and adsorption distances: Co on Cu(001). Physical Review B, 2018, 97, .	1.1	8
58	Current vortices in aromatic carbon molecules. Physical Review B, 2020, 102, .	1.1	8
59	Easy-plane to easy-axis anisotropy switching in a Co(<scp>ii</scp>) single-ion magnet triggered by the diamagnetic lattice. Journal of Materials Chemistry C, 2021, 9, 9446-9452.	2.7	8
60	2,2â€²â€Bipyridineâ€Based Dendritic Structured Compounds for Second Harmonic Generation. Chemistry - A European Journal, 2014, 20, 14351-14361.	1.7	6
61	GenLocDip: A Generalized Program to Calculate and Visualize Local Electric Dipole Moments. Journal of Computational Chemistry, 2016, 37, 2324-2334.	1.5	6
62	Limits of Molecular Dithienylethene Switches Caused by Ferrocenyl Substitution. ChemPhysChem, 2016, 17, 1881-1894.	1.0	6
63	Structural diradical character. Journal of Computational Chemistry, 2019, 40, 854-865.	1.5	6
64	Local electric dipole moments: A generalized approach. Journal of Computational Chemistry, 2016, 37, 2260-2265.	1.5	5
65	Why Are Dithienyletheneâ€Linked Biscobaltocenes so Hard to Photoswitch?. ChemPhysChem, 2017, 18, 596-609.	1.0	5
66	Synthesis, characterization and magnetic properties of head-to-head stacked vanadocenes. Dalton Transactions, 2017, 46, 15494-15502.	1.6	4
67	Hydrogen-bonded supramolecular metal-imidazolate frameworks: gas sorption, magnetic and UV/Vis spectroscopic properties. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2019, 94, 155-165.	0.9	4
68	Co(CO)n/Cu(001): Towards understanding chemical control of the Kondo effect. Journal of Applied Physics, 2019, 125, 142910.	1.1	4
69	Toward a First-Principles Evaluation of Transport Mechanisms in Molecular Wires. Journal of Chemical Theory and Computation, 2020, 16, 6267-6279.	2.3	4
70	EXAFS simulation refinement based on broken-symmetry DFT geometries for the Mn(<scp>iv</scp>)â€“Fe(<scp>iii</scp>) center of class I RNR from Chlamydia trachomatis. Dalton Transactions, 2014, 43, 576-583.	1.6	3
71	Modeling adsorbateâ€induced property changes of carbon nanotubes. Journal of Computational Chemistry, 2017, 38, 861-868.	1.5	3
72	Exchange Spin Coupling in Optically Excited States. Journal of Chemical Theory and Computation, 2022, 18, 4708-4718.	2.3	3

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73	Extended Threefoldâ€Symmetric Secondâ€Harmonicâ€Generation Chromophores Based on 1,3,5â€Trisubstituted Benzene Complexes. European Journal of Inorganic Chemistry, 2015, 2015, .	1.0	2
74	Controlling Throughâ€Space and Throughâ€Bond Exchange Pathways in Bisâ€Cobaltocenes for Molecular Spintronics. Angewandte Chemie, 2020, 132, 2428-2434.	1.6	2
75	Local decomposition of hybridization functions: Chemical insight into correlated molecular adsorbates. Journal of Chemical Physics, 2021, 154, 144108.	1.2	2
76	The angular dependence of spin-state energy splittings in the core. Molecular Physics, 2013, 111, 1482-1491.	0.8	1
77	Designing and Understanding Building Blocks for Molecular Spintronics. Nanoscience and Technology, 2018, , 117-136.	1.5	1
78	Rashba Spin-Orbit Coupling in Colloidal Lead Sulfide Nanosheets. , 2017, , .		1
79	Why Are Dithienyletheneâ€Linked Biscobaltocenes so Hard to Photoswitch?. ChemPhysChem, 2017, 18, 578-578.	1.0	0