Carmen Herrmann

List of Publications by Citations

77 papers	1,959 citations	23 h-index	42 g-index
96 ext. papers	2,205 ext. citations	5.2 avg, IF	5.07 L-index

#	Paper	IF	Citations
77	Exploring local currents in molecular junctions. *Nature Chemistry*, **2010**, 2, 223-8	17.6	325
76	Organic radicals as spin filters. *Journal of the American Chemical Society*, **2010**, 132, 3682-4	16.4	149
75	Ghost transmission: How large basis sets can make electron transport calculations worse. *Journal of Chemical Physics*, **2010**, 132, 024103	3.9	78
74	Comparative analysis of local spin definitions. *Journal of Chemical Physics*, **2005**, 122, 34102	3.9	77
73	Can Raman optical activity separate axial from local chirality? A theoretical study of helical deca-alanine. *ChemPhysChem*, **2006**, 7, 2189-96	3.2	69
72	The chameleonic nature of electron transport through pi-stacked systems. *Journal of the American Chemical Society*, **2010**, 132, 7887-9	16.4	68
71	Trinuclear copper(II) complexes derived from Schiff-base ligands based on a 6-amino-6-deoxyglucopyranoside: structural and magnetic characterization. *Inorganic Chemistry*, **2006**, 45, 10066-76	5.1	60
70	Finding a needle in a haystack: direct determination of vibrational signatures in complex systems. *New Journal of Chemistry*, **2007**, 31, 818	3.6	57
69	First-Principles Approach to Vibrational Spectroscopy of Biomolecules **2006**, 85-132		52
68	Large Magnetoresistance in Single-Radical Molecular Junctions. *Nano Letters*, **2016**, 16, 4960-7	11.5	50
67	M(O)V(I)P(AC): vibrational spectroscopy with a robust meta-program for massively parallel standard and inverse calculations. *Journal of Computational Chemistry*, **2012**, 33, 2186-98	3.5	50
66	The first photoexcitation step of ruthenium-based models for artificial photosynthesis highlighted by resonance Raman spectroscopy. *Journal of Physical Chemistry B*, **2007**, 111, 6078-87	3.4	50
65	Spin states in polynuclear clusters: the [Fe2O2] core of the methane monooxygenase active site. *Journal of Computational Chemistry*, **2006**, 27, 1223-39	3.5	50
64	Relevance of the electric-dipole--electric-quadrupole contribution to Raman optical activity spectra. *Journal of Physical Chemistry B*, **2008**, 112, 2218-32	3.4	45
63	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, 10078-87	4.8	45
62	Designing organic spin filters in the coherent tunneling regime. *Journal of Chemical Physics*, **2011**, 134, 224306	3.9	42
61	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	6.4	35

60	Spin–Spin interactions in polynuclear transition-metal complexes. *Chemical Physics Letters*, **2008**, 451, 301-308	2.5	34
59	Importance of backbone angles versus amino acid configurations in peptide vibrational Raman optical activity spectra. *Chemical Physics*, **2008**, 343, 200-209	2.3	31
58	Electronic communication through molecular bridges. *Chemical Communications*, **2013**, 49, 10456-8	5.8	29
57	Theoretical study on the spin-state energy splittings and local spin in cationic [Re]-Cn-[Re] complexes. *Inorganic Chemistry*, **2005**, 44, 6174-82	5.1	26
56	Understanding coherent transport through π-stacked systems upon spatial dislocation. *Journal of Physical Chemistry B*, **2010**, 114, 14735-44	3.4	25
55	Optical and vibrational properties of toroidal carbon nanotubes. *Chemistry - A European Journal*, **2011**, 17, 3868-75	4.8	23
54	Restrained optimization of broken-symmetry determinants. *International Journal of Quantum Chemistry*, **2009**, 109, 2430-2446	2.1	23
53	A Green's-Function Approach to Exchange Spin Coupling As a New Tool for Quantum Chemistry. *Journal of Chemical Theory and Computation*, **2015**, 11, 5651-64	6.4	21
52	Cobalt-Catalyzed Hydrogenations via Olefin Cobaltate and Hydride Intermediates. *ACS Catalysis*, **2019**, 9, 7596-7606	13.1	21
51	Controlling molecular conductance: switching off π-sites through protonation. *ChemPhysChem*, **2014**, 15, 4011-8	3.2	21
50	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	3.8	20
49	Molecular electronic junction transport: some pathways and some ideas. *Topics in Current Chemistry* , **2012**, 313, 1-38		20
48	QM/MM vibrational mode tracking. *Journal of Computational Chemistry*, **2008**, 29, 2460-70	3.5	20
47	Towards colloidal spintronics through Rashba spin-orbit interaction in lead sulphide nanosheets. *Nature Communications*, **2017**, 8, 15721	17.4	19
46	Communication through molecular bridges: different bridge orbital trends result in common property trends. *Journal of Computational Chemistry*, **2015**, 36, 201-9	3.5	18
45	Increasing Magnetic Coupling through Oxidation of a Ferrocene Bridge. *Inorganic Chemistry*, **2015**, 54, 11733-40	5.1	17
44	Direct targeting of adsorbate vibrations with mode-tracking. *Surface Science*, **2006**, 600, 1891-1900	1.8	17
43	High-conductance surface-anchoring of a mechanically flexible platform-based porphyrin complex. *New Journal of Physics*, **2015**, 17, 013012	2.9	16

42	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	6.4	16
41	Electronic Communication as a Transferable Property of Molecular Bridges?. *Journal of Physical Chemistry A*, **2019**, 123, 10205-10223	2.8	15
40	Charge delocalization in an organic mixed valent bithiophene is greater than in a structurally analogous biselenophene. *Journal of Physical Chemistry A*, **2014**, 118, 11293-303	2.8	14
39	Influence of Radical Bridges on Electron Spin Coupling. *Journal of Physical Chemistry A*, **2017**, 121, 216-225	2.8	12
38	Synthesis and Molecular Structures of Monosubstituted Pentamethylcobaltocenium Cations. *European Journal of Inorganic Chemistry*, **2014**, 2014, 4115-4122	2.3	12
37	Quantum Chemical Calculations and Experimental Validation of the Photoclick Reaction for Fluorescent Labeling of the 5R cap of Eukaryotic mRNAs. *ChemistryOpen*, **2015**, 4, 295-301	2.3	12
36	Mode-tracking based stationary-point optimization. *Journal of Computational Chemistry*, **2015**, 36, 1429-38	3.5	11
35	Synthesis, Structures, and Magnetic Properties of N-Trialkylsilyl-8-amidoquinoline Complexes of Chromium, Manganese, Iron, and Cobalt as well as of Wheel-Like Hexanuclear Iron(II) and Manganese(II) Bis(8-amidoquinoline). *European Journal of Inorganic Chemistry*, **2010**, 2010, 1777-1790	2.3	10
34	Performance of range-separated hybrid exchange-correlation functionals for the calculation of magnetic exchange coupling constants of organic diradicals. *Journal of Computational Chemistry*, **2018**, 39, 780-787	3.5	9
33	Toward an automated analysis of exchange pathways in spin-coupled systems. *Journal of Computational Chemistry*, **2018**, 39, 81-92	3.5	9
32	Interplay between strong correlation and adsorption distances: Co on Cu(001). *Physical Review B*, **2018**, 97,	3.3	8
31	Exchange Spin Coupling from Gaussian Process Regression. *Journal of Physical Chemistry A*, **2020**, 124, 8708-8723	2.8	8
30	Simultaneous manifestation of metallic conductivity and single-molecule magnetism in a layered molecule-based compound. *Chemical Science*, **2020**, 11, 11154-11161	9.4	8
29	Designing Long-Range Charge Delocalization from First-Principles. *Journal of Chemical Theory and Computation*, **2019**, 15, 165-177	6.4	8
28	Photoswitching Behavior of a Cyclohexene-Bridged versus a Cyclopentene-Bridged Dithienylethene System. *ChemPhysChem*, **2015**, 16, 1491-501	3.2	7
27	Kondo screening in Co adatoms with full Coulomb interaction. *Physical Review Research*, **2020**, 2,	3.9	7
26	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	16.4	7
25	Design Considerations for Oligo(p-phenyleneethynylene) Organic Radicals in Molecular Junctions. *Journal of Physical Chemistry C*, **2021**, 125, 1208-1220	3.8	7

24	Limits of Molecular Dithienylethene Switches Caused by Ferrocenyl Substitution. *ChemPhysChem*, **2016**, 17, 1881-94	3.2	6
23	GenLocDip: A Generalized Program to Calculate and Visualize Local Electric Dipole Moments. *Journal of Computational Chemistry*, **2016**, 37, 2324-34	3.5	5
22	2,2RBipyridine-based dendritic structured compounds for second harmonic generation. *Chemistry - A European Journal*, **2014**, 20, 14351-61	4.8	5
21	Controlling Through-Space and Through-Bond Exchange Pathways in Bis-Cobaltocenes for Molecular Spintronics. *Angewandte Chemie - International Edition*, **2020**, 59, 2407-2413	16.4	5
20	Why Are Dithienylethene-Linked Biscobaltocenes so Hard to Photoswitch?. *ChemPhysChem*, **2017**, 18, 596-609	3.2	4
19	Co(CO)n/Cu(001): Towards understanding chemical control of the Kondo effect. *Journal of Applied Physics*, **2019**, 125, 142910	2.5	4
18	Structural diradical character. *Journal of Computational Chemistry*, **2019**, 40, 854-865	3.5	4
17	Modeling adsorbate-induced property changes of carbon nanotubes. *Journal of Computational Chemistry*, **2017**, 38, 861-868	3.5	3
16	Synthesis, characterization and magnetic properties of head-to-head stacked vanadocenes. *Dalton Transactions*, **2017**, 46, 15494-15502	4.3	3
15	Local electric dipole moments: A generalized approach. *Journal of Computational Chemistry*, **2016**, 37, 2260-5	3.5	3
14	EXAFS simulation refinement based on broken-symmetry DFT geometries for the Mn(IV)-Fe(III) center of class I RNR from Chlamydia trachomatis. *Dalton Transactions*, **2014**, 43, 576-83	4.3	3
13	Chiral-Induced Spin Selectivity: A Symmetry Analysis of Electronic Transmission		3
12	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	1.7	2
11	Extended Threefold-Symmetric Second-Harmonic-Generation Chromophores Based on 1,3,5-Trisubstituted Benzene Complexes. *European Journal of Inorganic Chemistry*, **2015**, 2015, n/a-n/a	2.3	2
10	Controlling Through-Space and Through-Bond Exchange Pathways in Bis-Cobaltocenes for Molecular Spintronics. *Angewandte Chemie*, **2020**, 132, 2428-2434	3.6	2
9	Toward a First-Principles Evaluation of Transport Mechanisms in Molecular Wires. *Journal of Chemical Theory and Computation*, **2020**, 16, 6267-6279	6.4	2
8	Current vortices in aromatic carbon molecules. *Physical Review B*, **2020**, 102,	3.3	2
7	Spectroscopic Investigation of a Metal-Metal-Bonded Fe Single-Molecule Magnet with an Isolated = / Giant-Spin Ground State. *Inorganic Chemistry*, **2021**, 60, 4610-4622	5.1	2

6	The angular dependence of spin-state energy splittings in the core. *Molecular Physics*, **2013**, 111, 1482-1491	1.7	1
5	Rashba Spin-Orbit Coupling in Colloidal Lead Sulfide Nanosheets **2017**,		1
4	Local decomposition of hybridization functions: Chemical insight into correlated molecular adsorbates. *Journal of Chemical Physics*, **2021**, 154, 144108	3.9	1
3	Easy-plane to easy-axis anisotropy switching in a Co(II) single-ion magnet triggered by the diamagnetic lattice. *Journal of Materials Chemistry C*, **2021**, 9, 9446-9452	7.1	1
2	Designing and Understanding Building Blocks for Molecular Spintronics. *Nanoscience and Technology*, **2018**, 117-136	0.6	1
1	Why Are Dithienylethene-Linked Biscobaltocenes so Hard to Photoswitch?. *ChemPhysChem*, **2017**, 18, 578-578	3.2	