

Natalie Fey

List of Publications by Year in descending order

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77
papers

3,653
citations

94433

37
h-index

138484

58
g-index

90
all docs

90
docs citations

90
times ranked

3907
citing authors

#	ARTICLE	IF	CITATIONS
1	Computational Ligand Descriptors for Catalyst Design. <i>Chemical Reviews</i> , 2019, 119, 6561-6594.	47.7	254
2	Building ligand knowledge bases for organometallic chemistry: Computational description of phosphorus(III)-donor ligands and the metal–phosphorus bond. <i>Coordination Chemistry Reviews</i> , 2009, 253, 704-722.	18.8	180
3	Accurate modelling of Pd(0) + PhX oxidative addition kinetics. <i>Dalton Transactions</i> , 2010, 39, 10833.	3.3	179
4	A computational study of phosphine ligand effects in Suzuki–Miyaura coupling†. <i>Journal of Molecular Catalysis A</i> , 2010, 324, 39-47.	4.8	144
5	Expansion of the Ligand Knowledge Base for Monodentate P-Donor Ligands (LKB-P). <i>Organometallics</i> , 2010, 29, 6245-6258.	2.3	117
6	Development of a Ligand Knowledge Base, Part 1: Computational Descriptors for Phosphorus Donor Ligands. <i>Chemistry - A European Journal</i> , 2006, 12, 291-302.	3.3	110
7	The contribution of computational studies to organometallic catalysis: descriptors, mechanisms and models. <i>Dalton Transactions</i> , 2010, 39, 296-310.	3.3	109
8	Insights into the Mechanistic Basis of Plasmid-Mediated Colistin Resistance from Crystal Structures of the Catalytic Domain of MCR-1. <i>Scientific Reports</i> , 2017, 7, 39392.	3.3	107
9	Computed ligand effects on the oxidative addition of phenyl halides to phosphine supported palladium(0) catalysts. <i>Dalton Transactions</i> , 2014, 43, 13545-13556.	3.3	100
10	Counterintuitive Kinetics in Tsuji-Trost Allylation: Ion-Pair Partitioning and Implications for Asymmetric Catalysis. <i>Journal of the American Chemical Society</i> , 2008, 130, 14471-14473.	13.7	97
11	Computational Descriptors for Chelating P,P- and P,N-Donor Ligands ¹ . <i>Organometallics</i> , 2008, 27, 1372-1383.	2.3	96
12	The performance of nonhybrid density functionals for calculating the structures and spin states of Fe(II) and Fe(III) complexes. <i>Journal of Computational Chemistry</i> , 2004, 25, 1840-1848.	3.3	86
13	DommiMOE: An implementation of ligand field molecular mechanics in the molecular operating environment. <i>Journal of Computational Chemistry</i> , 2005, 26, 123-130.	3.3	76
14	Remarkably reactive dihydroindoloindoles via palladium-catalysed dearomatization. <i>Chemical Communications</i> , 2011, 47, 3649.	4.1	74
15	A Simple and Broadly Applicable C–N Bond Forming Dearomatization Protocol Enabled by Bifunctional Amino Reagents. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 14531-14535.	13.8	70
16	Expansion of the Ligand Knowledge Base for Chelating P,P-Donor Ligands (LKB-PP). <i>Organometallics</i> , 2012, 31, 5302-5306.	2.3	69
17	Functional block-like structures from electroactive tetra(aniline) oligomers. <i>Journal of Materials Chemistry</i> , 2011, 21, 18137.	6.7	67
18	Inclusion of the ligand field contribution in a polarizable molecular mechanics: SIBFA-LF. <i>Journal of Computational Chemistry</i> , 2003, 24, 1963-1970.	3.3	65

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19	Photophysical Properties of Platinum(II) Acetylide Complexes: the Effect of a Strongly Electron-Accepting Diimine Ligand on Excited-State Structure. <i>Inorganic Chemistry</i> , 2008, 47, 8242-8257.	4.0	65
20	Structural Fluctuations in Enzyme-Catalyzed Reactions: Determinants of Reactivity in Fatty Acid Amide Hydrolase from Multivariate Statistical Analysis of Quantum Mechanics/Molecular Mechanics Paths. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2948-2960.	5.3	61
21	A ligand knowledge base for carbenes (LKB-C): maps of ligand space. <i>Dalton Transactions</i> , 2009, , 8183.	3.3	59
22	Organometallic reactivity: the role of metal–ligand bond energies from a computational perspective. <i>Dalton Transactions</i> , 2011, 40, 11184.	3.3	57
23	The Computational Road to Better Catalysts. <i>Chemistry - an Asian Journal</i> , 2014, 9, 1714-1723.	3.3	57
24	Self-Assembly of a Functional Oligo(Aniline)-Based Amphiphile into Helical Conductive Nanowires. <i>Journal of the American Chemical Society</i> , 2015, 137, 14288-14294.	13.7	57
25	Heavily Substituted Atropisomeric Diarylamines by Unactivated Smiles Rearrangement of <i>N</i> -Aryl Anthranilamides. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 12533-12537.	13.8	57
26	Regioselective B-Cyclometalation of a Bulky <i>o</i> -Carboranyl Phosphine and the Unexpected Formation of a Dirhodium(II) Complex. <i>Organometallics</i> , 2012, 31, 2907-2913.	2.3	55
27	Computational Discovery of Stable Transition-Metal Vinylidene Complexes. <i>Organometallics</i> , 2014, 33, 1751-1761.	2.3	51
28	Near-Infrared Luminescence from Platinum(II) Diimine Compounds. <i>Inorganic Chemistry</i> , 2006, 45, 6105-6107.	4.0	50
29	Palladium Complexes of the Heterodiphosphine <i>o</i> -C ₆ H ₄ (CH ₂) ₂ P ^t Bu ₂ (CH) ₂ PPh ₂ Are Highly Selective and Robust Catalysts for the Hydromethoxycarbonylation of Ethene. <i>Organometallics</i> , 2010, 29, 2292-2305.	2.3	49
30	Cooperative Lewis Pairs Based on Late Transition Metals: Activation of Small Molecules by Platinum(0) and B(C ₆ F ₅) ₃ . <i>Angewandte Chemie - International Edition</i> , 2015, 54, 2223-2227.	13.8	49
31	Effect of fluorine and trifluoromethyl substitution on the donor properties and stereodynamical behaviour of triarylphosphines. <i>Journal of the Chemical Society Dalton Transactions</i> , 1999, , 3015-3028.	1.1	48
32	Stable Fluorophosphines: Predicted and Realized Ligands for Catalysis. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 118-122.	13.8	46
33	Visible-Light-Driven Strain-Increase Ring Contraction Allows the Synthesis of Cyclobutyl Boronic Esters. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 6525-6528.	13.8	46
34	Delineating Poly(Aniline) Redox Chemistry by Using Tailored Oligo(Aryleneamine)s: Towards Oligo(Aniline)-Based Organic Semiconductors with Tunable Optoelectronic Properties. <i>Chemistry - A European Journal</i> , 2011, 17, 12512-12521.	3.3	45
35	Synthesis, structures and properties of a new series of platinum–diimine–dithiolate complexes. <i>Dalton Transactions</i> , 2007, , 4446.	3.3	42
36	Building a Toolbox for the Analysis and Prediction of Ligand and Catalyst Effects in Organometallic Catalysis. <i>Accounts of Chemical Research</i> , 2021, 54, 837-848.	15.6	41

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37	Lost in chemical space? Maps to support organometallic catalysis. <i>Chemistry Central Journal</i> , 2015, 9, 38.	2.6	39
38	Anatomy of Phobanes. Diastereoselective Synthesis of the Three Isomers of <i>n</i> -Butylphobane and a Comparison of their Donor Properties. <i>Journal of the American Chemical Society</i> , 2009, 131, 3078-3092.	13.7	38
39	Organometallic molecular modelling - the computational chemistry of metallocenes: a review. , 1999, 74, 852-862.		36
40	Biocatalytic Routes to Lactone Monomers for Polymer Production. <i>Biochemistry</i> , 2018, 57, 1997-2008.	2.5	33
41	Accessing Alkyl- and Alkenylcyclopentanes from Cr-Catalyzed Ethylene Oligomerization Using 2-Phosphinophosphinine Ligands. <i>Organometallics</i> , 2018, 37, 1062-1073.	2.3	32
42	How Big is the Pinacol Boronic Ester as a Substituent?. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 22403-22407.	13.8	32
43	Screening substituent and backbone effects on the properties of bidentate P,P-donor ligands (LKB-PP _{screen}). <i>Dalton Transactions</i> , 2013, 42, 172-181.	3.3	30
44	Statistical Modeling of a Ligand Knowledge Base. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 2591-2600.	5.4	27
45	Cryptocatalytic 1,2-Alkene Migration in a η^5 -Alkyl Palladium Diene Complex. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 6262-6265.	13.8	27
46	Conformational Properties of Substituted Ferrocenes: An Experimental and Theoretical Studies of the Molecular Structures of 1,1'-Di- <i>tert</i> -butylferrocene and Isopropylferrocene. <i>Organometallics</i> , 2001, 20, 2309-2320.	2.3	26
47	Computational study of PtBu ₃ as ligand in the palladium-catalysed amination of phenylbromide with morpholine [†] . <i>Journal of Molecular Catalysis A</i> , 2010, 324, 48-55.	4.8	26
48	A Simple and Broadly Applicable C ^α -N Bond Forming Dearomatization Protocol Enabled by Bifunctional Amino Reagents. <i>Angewandte Chemie</i> , 2017, 129, 14723-14727.	2.0	20
49	Heavily Substituted Atropisomeric Diarylamines by Unactivated Smiles Rearrangement of N-Aryl Anthranilamides. <i>Angewandte Chemie</i> , 2017, 129, 12707-12711.	2.0	20
50	Computational mapping of redox-switchable metal complexes based on ferrocene derivatives. <i>Chemical Communications</i> , 2019, 55, 7021-7024.	4.1	20
51	A Molecular Mechanics Study of Copper(II)-Catalyzed Asymmetric Diels-Alder Reactions. <i>Organometallics</i> , 2004, 23, 1042-1054.	2.3	19
52	A molecular mechanics approach to mapping the conformational space of diaryl and triarylphosphines. <i>Dalton Transactions</i> , 2006, , 5464.	3.3	19
53	Adding Value to Crystallographically-Derived Knowledge Bases. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 912-929.	5.4	18
54	Dispersion, solvent and metal effects in the binding of gold cations to alkynyl ligands: implications for Au(<i>scpi</i>) catalysis. <i>Chemical Communications</i> , 2015, 51, 9702-9705.	4.1	18

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55	Visible-Light-Driven Strain-Increase Ring Contraction Allows the Synthesis of Cyclobutyl Boronic Esters. <i>Angewandte Chemie</i> , 2020, 132, 6587-6590.	2.0	18
56	Mapping the properties of bidentate ligands with calculated descriptors (LKB-bid). <i>Dalton Transactions</i> , 2020, 49, 8169-8178.	3.3	18
57	Exploring Redox States, Doping and Ordering of Electroactive Star-Shaped Oligo(aniline)s. <i>Chemistry - A European Journal</i> , 2016, 22, 16950-16956.	3.3	15
58	Molecular Mechanics Analysis of Structure and Diastereoselectivity toward Lithiation in Amido- and \pm -Aminoferrocene Complexes. <i>Organometallics</i> , 2002, 21, 5272-5286.	2.3	14
59	Synthesis and spectroelectrochemistry of transition metal carbonyls with 1,1-bis(phosphino)metallocene ligands. <i>Journal of Organometallic Chemistry</i> , 2012, 712, 37-45.	1.8	14
60	On the Basicity of Carboranylphosphines. <i>Inorganic Chemistry</i> , 2019, 58, 14818-14829.	4.0	12
61	Iron Catalyzed Double Bond Isomerization: Evidence for an Fe ^I /Fe ^{III} Catalytic Cycle. <i>Chemistry - A European Journal</i> , 2021, 27, 5972-5977.	3.3	12
62	Catalytic mechanism of the colistin resistance protein MCR-1. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 3813-3819.	2.8	11
63	Resistance to the α -elastase antibiotic colistin: a single-zinc mechanism for phosphointermediate formation in MCR enzymes. <i>Chemical Communications</i> , 2020, 56, 6874-6877.	4.1	10
64	Computational Mapping of Dirhodium(II) Catalysts. <i>Chemistry - A European Journal</i> , 2021, 27, 2402-2409.	3.3	10
65	Inorganic Triphenylphosphine. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 15802-15806.	13.8	9
66	Setting P-Donor Ligands into Context: An Application of the Ligand Knowledge Base (LKB) Approach. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2015, 190, 706-714.	1.6	8
67	Computational mechanistic study in organometallic catalysis: Why prediction is still a challenge. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 0, , e1590.	14.6	8
68	How Big is the Pinacol Boronic Ester as a Substituent?. <i>Angewandte Chemie</i> , 2020, 132, 22589-22593.	2.0	7
69	Tipping the polaron-bipolaron balance: concentration and spin effects in doped oligo(aniline)s observed by UV-vis-NIR and TD-DFT. <i>Molecular Systems Design and Engineering</i> , 2019, 4, 103-109.	3.4	6
70	3 \AA - Axial vs 3 \AA - Equatorial: The τ^* Value Is a Robust Computational Measure of Substituent Steric Effects. <i>Journal of the American Chemical Society</i> , 2021, 143, 13573-13578.	13.7	6
71	Spectroscopic, structural and computational analysis of [Re(CO) ₃ (dippM)Br] ⁿ⁺ (dippM = 1,1-bis(diiso-propylphosphino)metallocene, M =) <i>J. Organomet. Chem.</i> 2019, 931, 1-10. 784314	1.0	6
72	Computational and theoretical approaches for mechanistic understanding: general discussion. <i>Faraday Discussions</i> , 2019, 220, 464-488.	3.2	3

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73	Inorganic Triphenylphosphine. <i>Angewandte Chemie</i> , 2018, 130, 16028-16032.	2.0	2
74	Inclusion of the ligand field contribution in a polarizable molecular mechanics: SIBFA-LF. <i>Journal of Computational Chemistry</i> , 2004, 25, 308-308.	3.3	1
75	Understanding unusual element-element bond formation and activation: general discussion. <i>Faraday Discussions</i> , 2019, 220, 376-385.	3.2	0
76	Physical methods for mechanistic understanding: general discussion. <i>Faraday Discussions</i> , 2019, 220, 144-178.	3.2	0
77	Visible-Light-Driven Strain-Increase Ring Contraction Allows the Synthesis of Cyclobutyl Boronic Esters (<i>Angew. Chem.</i> 16/2020). <i>Angewandte Chemie</i> , 2020, 132, 6694-6694.	2.0	0