Fernanda Duarte

List of Publications by Year in Descending Order

73 papers	1,613 citations	25 h-index	38 g-index
103 ext. papers	2,160 ext. citations	9.9 avg, IF	5.42 L-index

#	Paper	IF	Citations
73	Amino-oxetanes as amide isosteres by an alternative defluorosulfonylative coupling of sulfonyl fluorides.. *Nature Chemistry*, **2022**,	17.6	5
72	Direct catalytic asymmetric synthesis of -chiral bicyclo[1.1.1]pentanes. *Nature Communications*, **2021**, 12, 1644	17.4	6
71	Highly Active Halogen Bonding and Chalcogen Bonding Chloride Transporters with Non-Protonophoric Activity. *Chemistry - A European Journal*, **2021**, 27, 11738-11745	4.8	18
70	autodE: Automated Calculation of Reaction Energy Profiles—Application to Organic and Organometallic Reactions. *Angewandte Chemie*, **2021**, 133, 4312-4320	3.6	0
69	autodE: Automated Calculation of Reaction Energy Profiles- Application to Organic and Organometallic Reactions. *Angewandte Chemie - International Edition*, **2021**, 60, 4266-4274	16.4	15
68	Red-shifted tetra--halo-azobenzenes for photo-regulated transmembrane anion transport. *Organic and Biomolecular Chemistry*, **2021**, 19, 9058-9067	3.9	4
67	Selectivity in organocatalysis—from qualitative to quantitative predictive models. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1518	7.9	5
66	Discovery of SARS-CoV-2 M peptide inhibitors from modelling substrate and ligand binding. *Chemical Science*, **2021**, 12, 13686-13703	9.4	14
65	Mass spectrometry reveals potential of -lactams as SARS-CoV-2 M inhibitors. *Chemical Communications*, **2021**, 57, 1430-1433	5.8	17
64	A transferable active-learning strategy for reactive molecular force fields. *Chemical Science*, **2021**, 12, 10944-10955	9.4	7
63	Characterization of the Zwitterionic Intermediate in 1,1-Carboboration of Alkynes. *Angewandte Chemie*, **2020**, 132, 12831-12835	3.6	4
62	Tuning the anion binding properties of lanthanide receptors to discriminate nucleoside phosphates in a sensing array. *Chemical Science*, **2020**, 11, 3619-3628	9.4	29
61	: A Python Module and Web App for Automated Metallocage Construction and Host-Guest Characterization. *Journal of Chemical Information and Modeling*, **2020**, 60, 3546-3557	6.1	13
60	Atropisomerism in Diarylamines: Structural Requirements and Mechanisms of Conformational Interconversion. *Angewandte Chemie - International Edition*, **2020**, 59, 18670-18678	16.4	12
59	Host-Guest-Induced Electron Transfer Triggers Radical-Cation Catalysis. *Journal of the American Chemical Society*, **2020**, 142, 2134-2139	16.4	44
58	Dearomative Photocatalytic Construction of Bridged 1,3-Diazepanes. *Angewandte Chemie*, **2020**, 132, 4150-4159	3.6	8
57	Characterization of the Zwitterionic Intermediate in 1,1-Carboboration of Alkynes. *Angewandte Chemie - International Edition*, **2020**, 59, 12731-12735	16.4	9

56	Rationalizing the diverse reactivity of [1.1.1]propellane through □delocalization. *Chemical Science*, **2020**, 11, 4895-4903	9.4	11
55	Double and Triple Ionisation of Isocyanic Acid. *Scientific Reports*, **2020**, 10, 2288	4.9	1
54	Dearomative Photocatalytic Construction of Bridged 1,3-Diazepanes. *Angewandte Chemie - International Edition*, **2020**, 59, 4121-4130	16.4	34
53	Rationalizing the Activity of an "Artificial Diels-Alderase": Establishing Efficient and Accurate Protocols for Calculating Supramolecular Catalysis. *Journal of the American Chemical Society*, **2020**, 142, 1300-1310	16.4	48
52	Atropisomerism in Diarylamines: Structural Requirements and Mechanisms of Conformational Interconversion. *Angewandte Chemie*, **2020**, 132, 18829-18837	3.6	5
51	Harnessing Sulfinyl Nitrenes: A Unified One-Pot Synthesis of Sulfoximines and Sulfonimidamides. *Journal of the American Chemical Society*, **2020**, 142, 15445-15453	16.4	33
50	Reverse Polarity Reductive Functionalization of Tertiary Amides via a Dual Iridium-Catalyzed Hydrosilylation and Single Electron Transfer Strategy. *ACS Catalysis*, **2020**, 10, 11438-11447	13.1	18
49	Synergistic Noncovalent Catalysis Facilitates Base-Free Michael Addition. *Journal of the American Chemical Society*, **2020**, 142, 17743-17750	16.4	20
48	-Hydroboration-oxidation products in □steroids a hydroboration--hydroboration mechanism. *Chemical Science*, **2020**, 11, 12764-12768	9.4	1
47	Transmembrane anion transport mediated by halogen bonding and hydrogen bonding triazole anionophores. *Chemical Science*, **2020**, 11, 4722-4729	9.4	21
46	A General Route to Bicyclo[1.1.1]pentanes through Photoredox Catalysis. *ACS Catalysis*, **2019**, 9, 9568-9574	13.1	59
45	Relative Binding Energies Predict Crystallographic Binding Modes of Ethionamide Booster Lead Compounds. *Journal of Physical Chemistry Letters*, **2019**, 10, 2244-2249	6.4	5
44	Catalytic Asymmetric Synthesis of Cyclohexanes by Hydrogen Borrowing Annulations. *Angewandte Chemie - International Edition*, **2019**, 58, 12558-12562	16.4	32
43	The Energetic Significance of Metallophilic Interactions. *Angewandte Chemie - International Edition*, **2019**, 58, 12617-12623	16.4	40
42	The Energetic Significance of Metallophilic Interactions. *Angewandte Chemie*, **2019**, 131, 12747-12753	3.6	7
41	Catalytic Asymmetric Synthesis of Cyclohexanes by Hydrogen Borrowing Annulations. *Angewandte Chemie*, **2019**, 131, 12688-12692	3.6	15
40	Host-Guest Chemistry of Self-Assembled Hemi-Cage Systems: The Dramatic Effect of Lost Pre-Organization. *Israel Journal of Chemistry*, **2019**, 59, 257-266	3.4	4
39	Bio-inspired Domino oxa-Michael/Diels-Alder/oxa-Michael Dimerization of para-Quinols. *Angewandte Chemie - International Edition*, **2018**, 57, 6198-6202	16.4	12

38	Cation-□interactions in protein-ligand binding: theory and data-mining reveal different roles for lysine and arginine. *Chemical Science*, **2018**, 9, 2655-2665	9.4	120
37	Evolutionary repurposing of a sulfatase: A new Michaelis complex leads to efficient transition state charge offset. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, E7293-E7302	11.5	28
36	Stereospecific 1,3-H Transfer of Indenols Proceeds via Persistent Ion-Pairs Anchored by NH□□ Interactions. *Journal of the American Chemical Society*, **2018**, 140, 16740-16748	16.4	11
35	Bio-inspired Domino oxa-Michael/Diels□Alder/oxa-Michael Dimerization of para-Quinols. *Angewandte Chemie*, **2018**, 130, 6306-6310	3.6	5
34	Introduction to the Empirical Valence Bond Approach **2017**, 27-61		
33	EVB Simulations of the Catalytic Activity of Monoamine Oxidases: From Chemical Physics to Neurodegeneration **2017**, 199-231		
32	Total Synthesis of a Dimeric Thymol Derivative Isolated from Arnica sachalinensis. *Angewandte Chemie*, **2017**, 129, 6917-6921	3.6	0
31	Total Synthesis of a Dimeric Thymol Derivative Isolated from Arnica sachalinensis. *Angewandte Chemie - International Edition*, **2017**, 56, 6813-6817	16.4	8
30	Modelling Chemical Reactions Using Empirical Force Fields **2017**, 1-25		1
29	Using Empirical Valence Bond Constructs as Reference Potentials For High-Level Quantum Mechanical Calculations **2017**, 63-92		
28	Empirical Valence Bond Methods for Exploring Reaction Dynamics in the Gas Phase and in Solution **2017**, 93-119		
27	Empirical Valence-Bond Models Based on Polarizable Force Fields for Infrared Spectroscopy **2017**, 121-144		
26	Empirical Valence Bond Simulations of Biological Systems **2017**, 145-171		
25	The Empirical Valence Bond Approach as a Tool for Designing Artificial Catalysts **2017**, 173-198		
24	Deoxydehydration of vicinal diols and polyols catalyzed by pyridinium perrhenate salts. *Catalysis Science and Technology*, **2017**, 7, 5644-5649	5.5	17
23	Molecular Recognition in Asymmetric Counteranion Catalysis: Understanding Chiral Phosphate-Mediated Desymmetrization. *Journal of the American Chemical Society*, **2017**, 139, 8886-8896	16.4	40
22	**2017**,		4
21	Computing organic stereoselectivity - from concepts to quantitative calculations and predictions. *Chemical Society Reviews*, **2016**, 45, 6093-6107	58.5	124

20	Promiscuity in the Enzymatic Catalysis of Phosphate and Sulfate Transfer. *Biochemistry*, **2016**, 55, 3061-84	3.2	26
19	Mechanisms of histone lysine-modifying enzymes: A computational perspective on the role of the protein environment. *Journal of Molecular Graphics and Modelling*, **2016**, 67, 69-84	2.8	9
18	The Competing Mechanisms of Phosphate Monoester Dianion Hydrolysis. *Journal of the American Chemical Society*, **2016**, 138, 10664-73	16.4	40
17	Cooperative Electrostatic Interactions Drive Functional Evolution in the Alkaline Phosphatase Superfamily. *Journal of the American Chemical Society*, **2015**, 137, 9061-76	16.4	45
16	Expanding the Catalytic Triad in Epoxide Hydrolases and Related Enzymes. *ACS Catalysis*, **2015**, 5, 5702-5713	11.3	31
15	Resolving apparent conflicts between theoretical and experimental models of phosphate monoester hydrolysis. *Journal of the American Chemical Society*, **2015**, 137, 1081-93	16.4	82
14	Recent advances in QM/MM free energy calculations using reference potentials. *Biochimica Et Biophysica Acta - General Subjects*, **2015**, 1850, 954-965	4	49
13	Concerted or stepwise: how much do free-energy landscapes tell us about the mechanisms of elimination reactions?. *Journal of Organic Chemistry*, **2014**, 79, 1280-8	4.2	22
12	The alkaline hydrolysis of sulfonate esters: challenges in interpreting experimental and theoretical data. *Journal of Organic Chemistry*, **2014**, 79, 2816-28	4.2	24
11	Empirical valence bond simulations of the hydride transfer step in the monoamine oxidase B catalyzed metabolism of dopamine. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 3347-55	4.2	46
10	Force field independent metal parameters using a nonbonded dummy model. *Journal of Physical Chemistry B*, **2014**, 118, 4351-62	3.4	110
9	Catalytic Zinc Complexes for Phosphate Diester Hydrolysis. *Angewandte Chemie*, **2014**, 126, 8385-8389	3.6	5
8	Catalytic zinc complexes for phosphate diester hydrolysis. *Angewandte Chemie - International Edition*, **2014**, 53, 8246-50	16.4	40
7	Modeling catalytic promiscuity in the alkaline phosphatase superfamily. *Physical Chemistry Chemical Physics*, **2013**, 15, 11160-77	3.6	41
6	How does Pin1 catalyze the cis-trans prolyl peptide bond isomerization? A QM/MM and mean reaction force study. *Journal of Physical Chemistry B*, **2012**, 116, 12972-9	3.4	25
5	Insights on the mechanism of proton transfer reactions in amino acids. *Physical Chemistry Chemical Physics*, **2011**, 13, 7773-82	3.6	28
4	The mechanism of H2 activation by (amino)carbenes. *Journal of Physical Chemistry A*, **2011**, 115, 3050-9	2.8	31
3	The catalytic effect of water on the keto-enol tautomerisation reaction of thioformic acid. *Molecular Physics*, **2010**, 108, 1375-1384	1.7	16

2	Discovery of SARS-CoV-2 Mpro Peptide Inhibitors from Modelling Substrate and Ligand Binding		1
1	Computational Modeling of Supramolecular Metallo-organic Cages: Challenges and Opportunities. *ACS Catalysis*,5806-5826	13.1	3