

Fernanda Duarte

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Computing organic stereoselectivity - from concepts to quantitative calculations and predictions. <i>Chemical Society Reviews</i> , 2016 , 45, 6093-6107	58.5	124
72	Cation- π Interactions in protein-ligand binding: theory and data-mining reveal different roles for lysine and arginine. <i>Chemical Science</i> , 2018 , 9, 2655-2665	9.4	120
71	Force field independent metal parameters using a nonbonded dummy model. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 4351-62	3.4	110
70	Resolving apparent conflicts between theoretical and experimental models of phosphate monoester hydrolysis. <i>Journal of the American Chemical Society</i> , 2015 , 137, 1081-93	16.4	82
69	A General Route to Bicyclo[1.1.1]pentanes through Photoredox Catalysis. <i>ACS Catalysis</i> , 2019 , 9, 9568-9574	17.1	59
68	Recent advances in QM/MM free energy calculations using reference potentials. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2015 , 1850, 954-965	4	49
67	Rationalizing the Activity of an "Artificial Diels-Alderase": Establishing Efficient and Accurate Protocols for Calculating Supramolecular Catalysis. <i>Journal of the American Chemical Society</i> , 2020 , 142, 1300-1310	16.4	48
66	Empirical valence bond simulations of the hydride transfer step in the monoamine oxidase B catalyzed metabolism of dopamine. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014 , 82, 3347-55	4.2	46
65	Cooperative Electrostatic Interactions Drive Functional Evolution in the Alkaline Phosphatase Superfamily. <i>Journal of the American Chemical Society</i> , 2015 , 137, 9061-76	16.4	45
64	Host-Guest-Induced Electron Transfer Triggers Radical-Cation Catalysis. <i>Journal of the American Chemical Society</i> , 2020 , 142, 2134-2139	16.4	44
63	Modeling catalytic promiscuity in the alkaline phosphatase superfamily. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 11160-77	3.6	41
62	The Energetic Significance of Metallophilic Interactions. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 12617-12623	16.4	40
61	Molecular Recognition in Asymmetric Counteranion Catalysis: Understanding Chiral Phosphate-Mediated Desymmetrization. <i>Journal of the American Chemical Society</i> , 2017 , 139, 8886-8896	16.4	40
60	Catalytic zinc complexes for phosphate diester hydrolysis. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 8246-50	16.4	40
59	The Competing Mechanisms of Phosphate Monoester Dianion Hydrolysis. <i>Journal of the American Chemical Society</i> , 2016 , 138, 10664-73	16.4	40
58	Dearomative Photocatalytic Construction of Bridged 1,3-Diazepanes. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 4121-4130	16.4	34
57	Harnessing Sulfinyl Nitrenes: A Unified One-Pot Synthesis of Sulfoximines and Sulfonimidamides. <i>Journal of the American Chemical Society</i> , 2020 , 142, 15445-15453	16.4	33

56	Catalytic Asymmetric Synthesis of Cyclohexanes by Hydrogen Borrowing Annulations. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 12558-12562	16.4	32
55	Expanding the Catalytic Triad in Epoxide Hydrolases and Related Enzymes. <i>ACS Catalysis</i> , 2015 , 5, 5702-5713	3.1	31
54	The mechanism of H ₂ activation by (amino)carbenes. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 3050-9	2.8	31
53	Tuning the anion binding properties of lanthanide receptors to discriminate nucleoside phosphates in a sensing array. <i>Chemical Science</i> , 2020 , 11, 3619-3628	9.4	29
52	Evolutionary repurposing of a sulfatase: A new Michaelis complex leads to efficient transition state charge offset. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, E7293-E7302	11.5	28
51	Insights on the mechanism of proton transfer reactions in amino acids. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 7773-82	3.6	28
50	Promiscuity in the Enzymatic Catalysis of Phosphate and Sulfate Transfer. <i>Biochemistry</i> , 2016 , 55, 3061-8	3.2	26
49	How does Pin1 catalyze the cis-trans prolyl peptide bond isomerization? A QM/MM and mean reaction force study. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 12972-9	3.4	25
48	The alkaline hydrolysis of sulfonate esters: challenges in interpreting experimental and theoretical data. <i>Journal of Organic Chemistry</i> , 2014 , 79, 2816-28	4.2	24
47	Concerted or stepwise: how much do free-energy landscapes tell us about the mechanisms of elimination reactions?. <i>Journal of Organic Chemistry</i> , 2014 , 79, 1280-8	4.2	22
46	Transmembrane anion transport mediated by halogen bonding and hydrogen bonding triazole anionophores. <i>Chemical Science</i> , 2020 , 11, 4722-4729	9.4	21
45	Synergistic Noncovalent Catalysis Facilitates Base-Free Michael Addition. <i>Journal of the American Chemical Society</i> , 2020 , 142, 17743-17750	16.4	20
44	Reverse Polarity Reductive Functionalization of Tertiary Amides via a Dual Iridium-Catalyzed Hydrosilylation and Single Electron Transfer Strategy. <i>ACS Catalysis</i> , 2020 , 10, 11438-11447	13.1	18
43	Highly Active Halogen Bonding and Chalcogen Bonding Chloride Transporters with Non-Protonophoric Activity. <i>Chemistry - A European Journal</i> , 2021 , 27, 11738-11745	4.8	18
42	Deoxydehydration of vicinal diols and polyols catalyzed by pyridinium perchlorate salts. <i>Catalysis Science and Technology</i> , 2017 , 7, 5644-5649	5.5	17
41	Mass spectrometry reveals potential of lactams as SARS-CoV-2 M inhibitors. <i>Chemical Communications</i> , 2021 , 57, 1430-1433	5.8	17
40	The catalytic effect of water on the keto-enol tautomerisation reaction of thioformic acid. <i>Molecular Physics</i> , 2010 , 108, 1375-1384	1.7	16
39	Catalytic Asymmetric Synthesis of Cyclohexanes by Hydrogen Borrowing Annulations. <i>Angewandte Chemie</i> , 2019 , 131, 12688-12692	3.6	15

38	autodE: Automated Calculation of Reaction Energy Profiles- Application to Organic and Organometallic Reactions. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 4266-4274	16.4	15
37	Discovery of SARS-CoV-2 M peptide inhibitors from modelling substrate and ligand binding. <i>Chemical Science</i> , 2021 , 12, 13686-13703	9.4	14
36	: A Python Module and Web App for Automated Metallocage Construction and Host-Guest Characterization. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 3546-3557	6.1	13
35	Atropisomerism in Diarylamines: Structural Requirements and Mechanisms of Conformational Interconversion. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 18670-18678	16.4	12
34	Bio-inspired Domino oxa-Michael/Diels-Alder/oxa-Michael Dimerization of para-Quinols. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 6198-6202	16.4	12
33	Rationalizing the diverse reactivity of [1.1.1]propellane through π delocalization. <i>Chemical Science</i> , 2020 , 11, 4895-4903	9.4	11
32	Stereospecific 1,3-H Transfer of Indenols Proceeds via Persistent Ion-Pairs Anchored by NH \cdots Interactions. <i>Journal of the American Chemical Society</i> , 2018 , 140, 16740-16748	16.4	11
31	Characterization of the Zwitterionic Intermediate in 1,1-Carboboration of Alkynes. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 12731-12735	16.4	9
30	Mechanisms of histone lysine-modifying enzymes: A computational perspective on the role of the protein environment. <i>Journal of Molecular Graphics and Modelling</i> , 2016 , 67, 69-84	2.8	9
29	Total Synthesis of a Dimeric Thymol Derivative Isolated from <i>Arnica sachalinensis</i> . <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 6813-6817	16.4	8
28	Dearomative Photocatalytic Construction of Bridged 1,3-Diazepanes. <i>Angewandte Chemie</i> , 2020 , 132, 4150-4159	3.6	8
27	The Energetic Significance of Metallophilic Interactions. <i>Angewandte Chemie</i> , 2019 , 131, 12747-12753	3.6	7
26	A transferable active-learning strategy for reactive molecular force fields. <i>Chemical Science</i> , 2021 , 12, 10944-10955	9.4	7
25	Direct catalytic asymmetric synthesis of β chiral bicyclo[1.1.1]pentanes. <i>Nature Communications</i> , 2021 , 12, 1644	17.4	6
24	Relative Binding Energies Predict Crystallographic Binding Modes of Ethionamide Booster Lead Compounds. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 2244-2249	6.4	5
23	Catalytic Zinc Complexes for Phosphate Diester Hydrolysis. <i>Angewandte Chemie</i> , 2014 , 126, 8385-8389	3.6	5
22	Amino-oxetanes as amide isosteres by an alternative defluorosulfonylative coupling of sulfonyl fluorides.. <i>Nature Chemistry</i> , 2022 ,	17.6	5
21	Atropisomerism in Diarylamines: Structural Requirements and Mechanisms of Conformational Interconversion. <i>Angewandte Chemie</i> , 2020 , 132, 18829-18837	3.6	5

20	Selectivity in organocatalysis From qualitative to quantitative predictive models. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021 , 11, e1518	7.9	5
19	Bio-inspired Domino oxa-Michael/Diels-Alder/oxa-Michael Dimerization of para-Quinols. <i>Angewandte Chemie</i> , 2018 , 130, 6306-6310	3.6	5
18	Characterization of the Zwitterionic Intermediate in 1,1-Carboboration of Alkynes. <i>Angewandte Chemie</i> , 2020 , 132, 12831-12835	3.6	4
17	Host-Guest Chemistry of Self-Assembled Hemi-Cage Systems: The Dramatic Effect of Lost Pre-Organization. <i>Israel Journal of Chemistry</i> , 2019 , 59, 257-266	3.4	4
16	Red-shifted tetra-halo-azobenzenes for photo-regulated transmembrane anion transport. <i>Organic and Biomolecular Chemistry</i> , 2021 , 19, 9058-9067	3.9	4
15	2017 ,		4
14	Computational Modeling of Supramolecular Metallo-organic Cages Challenges and Opportunities. <i>ACS Catalysis</i> , 5806-5826	13.1	3
13	Modelling Chemical Reactions Using Empirical Force Fields 2017 , 1-25		1
12	Double and Triple Ionisation of Isocyanic Acid. <i>Scientific Reports</i> , 2020 , 10, 2288	4.9	1
11	-Hydroboration-oxidation products in Esters a hydroboration-hydroboration mechanism. <i>Chemical Science</i> , 2020 , 11, 12764-12768	9.4	1
10	Discovery of SARS-CoV-2 Mpro Peptide Inhibitors from Modelling Substrate and Ligand Binding		1
9	Total Synthesis of a Dimeric Thymol Derivative Isolated from <i>Arnica sachalinensis</i> . <i>Angewandte Chemie</i> , 2017 , 129, 6917-6921	3.6	0
8	autodE: Automated Calculation of Reaction Energy Profiles Application to Organic and Organometallic Reactions. <i>Angewandte Chemie</i> , 2021 , 133, 4312-4320	3.6	0
7	Introduction to the Empirical Valence Bond Approach 2017 , 27-61		
6	EVB Simulations of the Catalytic Activity of Monoamine Oxidases: From Chemical Physics to Neurodegeneration 2017 , 199-231		
5	Using Empirical Valence Bond Constructs as Reference Potentials For High-Level Quantum Mechanical Calculations 2017 , 63-92		
4	Empirical Valence Bond Methods for Exploring Reaction Dynamics in the Gas Phase and in Solution 2017 , 93-119		
3	Empirical Valence-Bond Models Based on Polarizable Force Fields for Infrared Spectroscopy 2017 , 121-144		

2 Empirical Valence Bond Simulations of Biological Systems **2017**, 145-171

1 The Empirical Valence Bond Approach as a Tool for Designing Artificial Catalysts **2017**, 173-198