Rachel Crespo-Otero

List of Publications by Citations

83 papers	1,978 citations	24 h-index	41 g-index
93 ext. papers	2,319 ext. citations	6.2 avg, IF	5.64 L-index

#	Paper	IF	Citations
83	Recent Advances and Perspectives on Nonadiabatic Mixed Quantum-Classical Dynamics. *Chemical Reviews*, **2018**, 118, 7026-7068	68.1	270
82	Spectrum simulation and decomposition with nuclear ensemble: formal derivation and application to benzene, furan and 2-phenylfuran. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	175
81	Surface Hopping Dynamics with Correlated Single-Reference Methods: 9H-Adenine as a Case Study. *Journal of Chemical Theory and Computation*, **2014**, 10, 1395-405	6.4	139
80	Exploring Potential Energy Surfaces for Aggregation-Induced Emission-From Solution to Crystal. *Chemistry - an Asian Journal*, **2019**, 14, 700-714	4.5	98
79	Critical appraisal of excited state nonadiabatic dynamics simulations of 9H-adenine. *Journal of Chemical Physics*, **2012**, 137, 22A503	3.9	90
78	Surface Hopping Dynamics with DFT Excited States. *Topics in Current Chemistry*, **2016**, 368, 415-44		48
77	Modelling a Linker Mix-and-Match Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks. *Angewandte Chemie - International Edition*, **2016**, 55, 16012-16016	16.4	47
76	How Inter- and Intramolecular Processes Dictate Aggregation-Induced Emission in Crystals Undergoing Excited-State Proton Transfer. *Journal of Physical Chemistry Letters*, **2017**, 8, 6148-6153	6.4	46
75	Excited state proton transfer in 2Shydroxychalcone derivatives. *Physical Chemistry Chemical Physics*, **2017**, 19, 2409-2416	3.6	44
74	Stepwise double excited-state proton transfer is not possible in 7-azaindole dimer. *Chemical Science*, **2015**, 6, 5762-5767	9.4	42
73	H-Center and V-Center Defects in Hybrid Halide Perovskites. *ACS Energy Letters*, **2017**, 2, 2713-2714	20.1	39
72	Influence of Density Functionals and Basis Sets on One-Bond Carbon-Carbon NMR Spin-Spin Coupling Constants. *Journal of Chemical Theory and Computation*, **2008**, 4, 448-56	6.4	38
71	Interfacial States in Donor-Acceptor Organic Heterojunctions: Computational Insights into Thiophene-Oligomer/Fullerene Junctions. *Journal of Chemical Theory and Computation*, **2013**, 9, 533-42	6.4	36
70	Ultrafast dynamics of UV-excited imidazole. *ChemPhysChem*, **2011**, 12, 3365-75	3.2	32
69	Interaction and reaction of the phenyl radical with water: a source of OH radicals. *Angewandte Chemie - International Edition*, **2009**, 48, 4804-7	16.4	32
68	Ultrafast Photoinduced Dynamics of 1,3-Cyclohexadiene Using XMS-CASPT2 Surface Hopping. *Journal of Chemical Theory and Computation*, **2019**, 15, 3929-3940	6.4	30
67	Variation in Surface Ionization Potentials of Pristine and Hydrated BiVO4. *Journal of Physical Chemistry Letters*, **2015**, 6, 2379-83	6.4	30

66	Basis set superposition error in MP2 and density-functional theory: a case of methane-nitric oxide association. *Journal of Chemical Physics*, **2005**, 123, 134107	3.9	30
65	Tunable optical properties of OH-functionalised graphene quantum dots. *Journal of Materials Chemistry C*, **2016**, 4, 8429-8438	7.1	27
64	Ab initio and matrix isolation study of the acetylene–furan dimer. *Chemical Physics*, **2008**, 343, 168-185	2.3	27
63	Steady and Time-Resolved Photoelectron Spectra Based on Nuclear Ensembles. *Journal of Chemical Theory and Computation*, **2016**, 12, 5037-5049	6.4	27
62	Endoplasmic reticulum targeting fluorescent probes to image mobile Zn. *Chemical Science*, **2019**, 10, 10881-10887	9.4	27
61	Interactions between simple radicals and water. *Chemical Physics*, **2008**, 353, 193-201	2.3	25
60	Cr(CO)6 photochemistry: semi-classical study of UV absorption spectral intensities and dynamics of photodissociation. *Journal of Chemical Physics*, **2011**, 134, 164305	3.9	24
59	Photochemistry and reactivity of the phenyl radical-water system: a matrix isolation and computational study. *Chemistry - A European Journal*, **2010**, 16, 8679-89	4.8	24
58	Band energy control of molybdenum oxide by surface hydration. *Applied Physics Letters*, **2015**, 107, 231605	3.4	23
57	New Insights into the State Trapping of UV-Excited Thymine. *Molecules*, **2016**, 21,	4.8	23
56	Solution-Processable Carbon Nanoelectrodes for Single-Molecule Investigations. *Journal of the American Chemical Society*, **2016**, 138, 2905-8	16.4	22
55	A novel in-silico approach for QSAR Studies of Anabolic and Androgenic Activities in the 17β-hydroxy-5α-androstane Steroid Family. *QSAR and Combinatorial Science*, **2005**, 24, 218-226		21
54	Computational NMR coupling constants: shifting and scaling factors for evaluating 1JCH. *Magnetic Resonance in Chemistry*, **2013**, 51, 775-87	2.1	18
53	Interactions of aromatic radicals with water. *ChemPhysChem*, **2013**, 14, 805-11	3.2	18
52	Photo-stability of peptide-bond aggregates: N-methylformamide dimers. *Physical Chemistry Chemical Physics*, **2014**, 16, 18877-87	3.6	17
51	Understanding rhodopsin mutations linked to the retinitis pigmentosa disease: a QM/MM and DFT/MRCI study. *Journal of Physical Chemistry B*, **2012**, 116, 1060-76	3.4	17
50	On the unusual 2J(C2-H(f)) coupling dependence on syn/anti CHO conformation in 5-X-furan-2-carboxaldehydes. *Magnetic Resonance in Chemistry*, **2008**, 46, 846-50	2.1	17
49	Applying pattern recognition methods plus quantum and physico-chemical molecular descriptors to analyze the anabolic activity of structurally diverse steroids. *Journal of Computational Chemistry*, **2008**, 29, 317-33	3.5	17

48	CNDOL: A fast and reliable method for the calculation of electronic properties of very large systems. Applications to retinal binding pocket in rhodopsin and gas phase porphine. *Journal of Chemical Physics*, **2007**, 127, 145102	3.9	17
47	ONIOM(QM:QM$) Electrostatic Embedding Schemes for Photochemistry in Molecular Crystals. *Journal of Chemical Theory and Computation*, **2019**, 15, 2504-2516	6.4	15
46	Molecular and crystalline requirements for solid state fluorescence exploiting excited state intramolecular proton transfer. *Journal of Materials Chemistry C*, **2020**, 8, 2558-2568	7.1	15
45	Biotin-tagged fluorescent sensor to visualize $mobile$Zn in cancer cells. *Chemical Communications*, **2018**, 54, 9619-9622	5.8	14
44	Patterns of retinal light absorption related to retinitis pigmentosa mutants from in silico model structures of rhodopsin. *Proteins: Structure, Function and Bioinformatics*, **2004**, 57, 392-9	4.2	14
43	Insights on the Auxochromic Properties of the Guanidinium Group. *Journal of Physical Chemistry A*, **2016**, 120, 7088-100	2.8	13
42	Organic room-temperature phosphorescence from halogen-bonded organic frameworks: hidden electronic effects in rigidified chromophores. *Chemical Science*, **2020**, 12, 767-773	9.4	13
41	Understanding Aggregation Induced Emission in a Propeller-Shaped Blue Emitter. *ChemPhotoChem*, **2019**, 3, 907-915	3.3	12
40	Energetics, thermal isomerisation and photochemistry of the linkage-isomer system [Ni(Et4dien)(κ2-O,ON)(κ1-NO2)]. *CrystEngComm*, **2015**, 17, 383-394	3.3	12
39	Photochemistry of N-methylformamide: matrix isolation and nonadiabatic dynamics. *ChemPhysChem*, **2013**, 14, 827-36	3.2	12
38	Intermolecular Aryne Ene Reaction of Hantzsch Esters: Stable Covalent Ene Adducts from a 1,4-Dihydropyridine Reaction. *Organic Letters*, **2017**, 19, 4644-4647	6.2	11
37	Karplus Equation for (3)JHH Spin-Spin Couplings with Unusual (3)J(180°) Journal of Chemical Theory and Computation, **2008**, 4, 1494-500	6.4	11
36	Exploring the potential energy surfaces of association of NO with aminoacids and related organic functional groups: the role of entropy of association. *Theoretical Chemistry Accounts*, **2007**, 118, 649-663	1.9	11
35	Chemometric and chemoinformatic analyses of anabolic and androgenic activities of testosterone and dihydrotestosterone analogues. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 6448-59	3.4	11
34	Electronic excitations in molecular solids: bridging theory and experiment. *Faraday Discussions*, **2015**, 177, 181-202	3.6	10
33	NMR spin–spin coupling constants and hyperconjugative interactions. *International Journal of Quantum Chemistry*, **2010**, 110, 532-539	2.1	10
32	fromage: A library for the study of molecular crystal excited states at the aggregate scale. *Journal of Computational Chemistry*, **2020**, 41, 1045-1058	3.5	10
31	Potential energy surfaces and Jahn-Teller effect on CH4...NO complexes. *Journal of Chemical Physics*, **2007**, 127, 104305	3.9	9

30	Quantitative Structure–Activity Relationship of the 4,5-Dihydrotestosterone Steroid Family. *QSAR and Combinatorial Science*, **2006**, 25, 881-894		9
29	Interaction and Reaction of the Phenyl Radical with Water: A Source of OH Radicals. *Angewandte Chemie*, **2009**, 121, 4898-4901	3.6	8
28	Theoretical model of internal rotation in monosubstituted derivatives of furfural. *Journal of Computational Chemistry*, **2004**, 25, 429-38	3.5	8
27	Synthesis of graphene mesosponge via catalytic methane decomposition on magnesium oxide. *Journal of Materials Chemistry A*, **2021**, 9, 14296-14308	13	8
26	Role of Conical Intersections on the Efficiency of Fluorescent Organic Molecular Crystals. *Journal of Physical Chemistry A*, **2021**, 125, 1012-1024	2.8	8
25	Communication: Accurate determination of side-chain torsion angle χ1 in proteins: phenylalanine residues. *Journal of Chemical Physics*, **2011**, 134, 061101	3.9	7
24	Water oxidation catalysed by quantum-sized BiVO4. *Journal of Materials Chemistry A*, **2018**, 6, 24965-24970	13	7
23	Aggregation-Induced Emission in the Tetraphenylthiophene Crystal: The Role of Triplet States. *Journal of Physical Chemistry C*, **2020**, 124, 17752-17761	3.8	6
22	Rotaxane Co Complexes as Field-Induced Single-Ion Magnets. *Angewandte Chemie - International Edition*, **2021**, 60, 16051-16058	16.4	6
21	An alternative modular 'click-SAr-click' approach to develop subcellular localised fluorescent probes to image mobile Zn . *Organic and Biomolecular Chemistry*, **2019**, 17, 10013-10019	3.9	6
20	Electronic structure of fullerene-squaraine complexes for photovoltaic devices. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 237-242	2	5
19	Excited state mechanisms in crystalline carbazole: the role of aggregation and isomeric defects. *Journal of Materials Chemistry C*, **2021**, 9, 11882-11892	7.1	5
18	Switching the Spin State of Pentafluorophenylnitrene: Isolation of a Singlet Arylnitrene Complex. *Journal of the American Chemical Society*, **2018**, 140, 17271-17277	16.4	5
17	Guanidine and guanidinium cation in the excited state--theoretical investigation. *Journal of Chemical Physics*, **2014**, 141, 074307	3.9	4
16	Aryne-Mediated Arylation of Hantzsch Esters: Access to Highly Substituted Aryl-dihydropyridines, Aryl-tetrahydropyridines and Spiro[benzocyclobutene-1,1?-(3?,4?-dihydropyridines)]. *Synthesis*, **2018**, 50, 4591-4605	2.9	4
15	Theoretical DFT karplus equations: Amino acid side-chain torsion angle χ1. *International Journal of Quantum Chemistry*, **2013**, 113, 656-660	2.1	3
14	Engineering the electronic and optical properties of 2D porphyrin-paddlewheel metal-organic frameworks. *JPhys Energy*, **2021**, 3, 034005	4.9	3
13	Theoretical study of imidazole...NO complexes. *Journal of Physical Chemistry A*, **2009**, 113, 14595-605	2.8	2

12	Influence of diosgenin structure on the polymerization kinetics of acrylamide: An experimental and theoretical approach. *Journal of Molecular Structure*, **2011**, 985, 34-47	3.4	2
11	Molecular orbital model of the influence of interaction between O2 and aluminosilicate sites on the triplet-singlet energy gap and reactivity. *Journal of Molecular Graphics and Modelling*, **2010**, 28, 746-54	2.8	2
10	Theoretical study of m-dansylaminophenylboronic acid and their species: A sugar chemosensor. *Computational and Theoretical Chemistry*, **2008**, 852, 71-77		2
9	Spectrum simulation and decomposition with nuclear ensemble: formal derivation and application to benzene, furan and 2-phenylfuran. *Highlights in Theoretical Chemistry*, **2014**, 89-102		2
8	Conformational and NMR study of some furan derivatives by DFT methods. *Journal of Molecular Modeling*, **2013**, 19, 4591-601	2	1
7	Rotaxane CoII Complexes as Field-Induced Single-Ion Magnets. *Angewandte Chemie*, **2021**, 133, 16187-16194	3.6	1
6	Protect to detect: A Golgi apparatus targeted probe to image mobile zinc through the use of a lipophilic cell-labile protecting group strategy. *Sensors and Actuators B: Chemical*, **2021**, 338, 129850	8.5	1
5	Porous nanographene formation on □alumina nanoparticles transition-metal-free methane activation.. *Chemical Science*, **2022**, 13, 3140-3146	9.4	1
4	A Global Potential Energy Surface Approach to the Photophysics of AIEgens **2022**, 411-454		1
3	Complexes of nitric oxide with water and imidazole. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	0
2	Triplet Generation Dynamics in Si- and Ge-Bridged Conjugated Copolymers. *Journal of Physical Chemistry C*, **2022**, 126, 1036-1045	3.8	0
1	Inside Cover: Photochemistry and Reactivity of the Phenyl Radical□Water System: A Matrix Isolation and Computational Study (Chem. Eur. J. 29/2010). *Chemistry - A European Journal*, **2010**, 16, 8566-8566	4.8	